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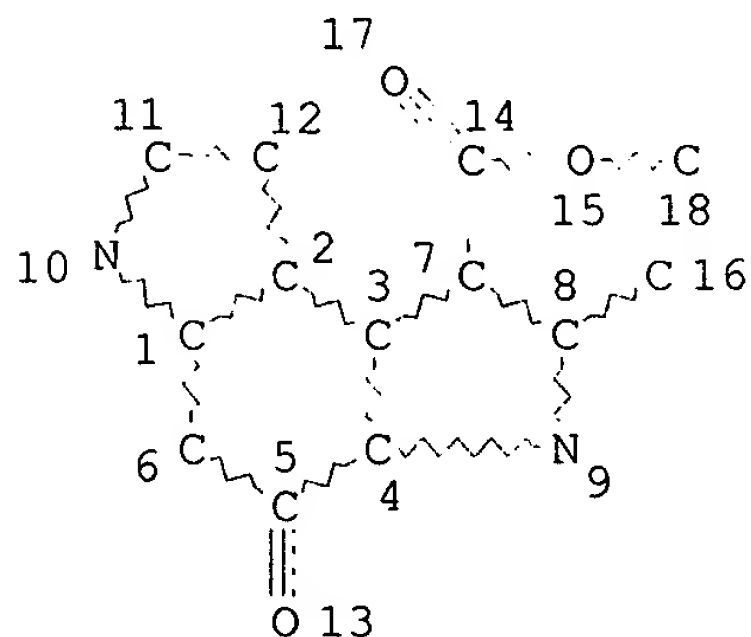
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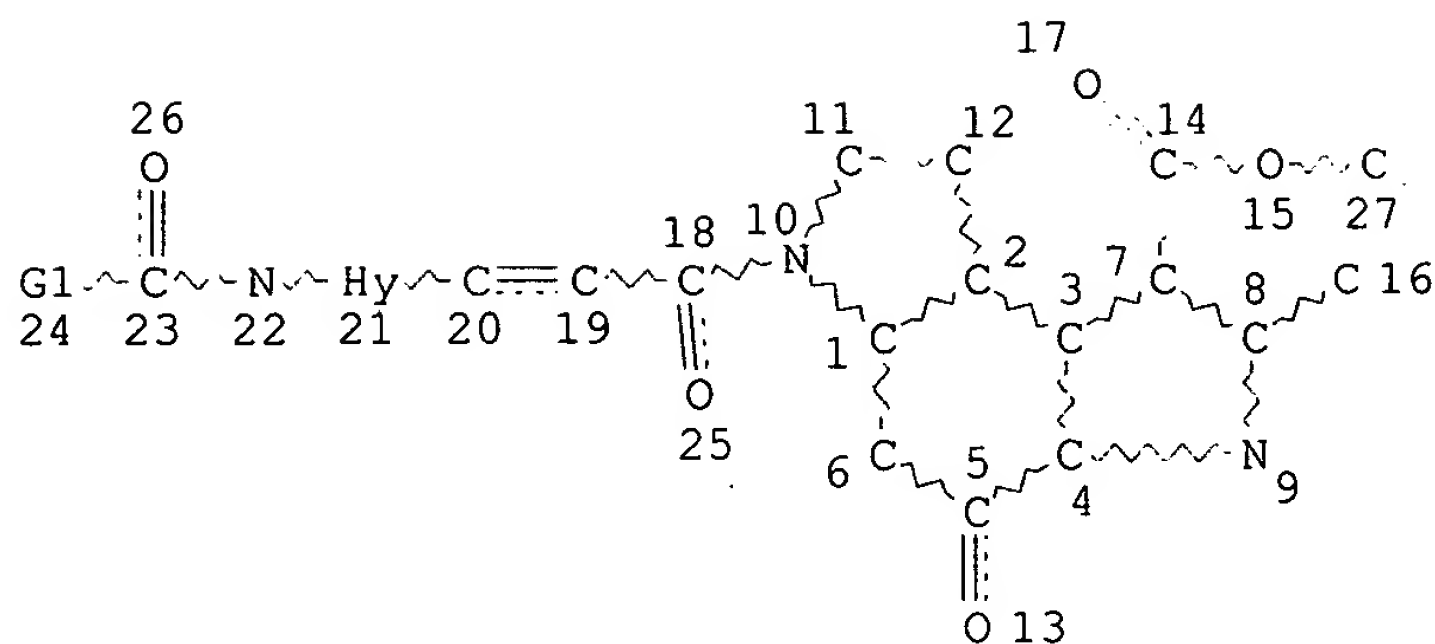
=> d stat que 112
 L7 STR



NODE ATTRIBUTES:
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
 L9 189 SEA FILE=REGISTRY SSS FUL L7
 L10 STR



VAR G1=C/CY.
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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 27

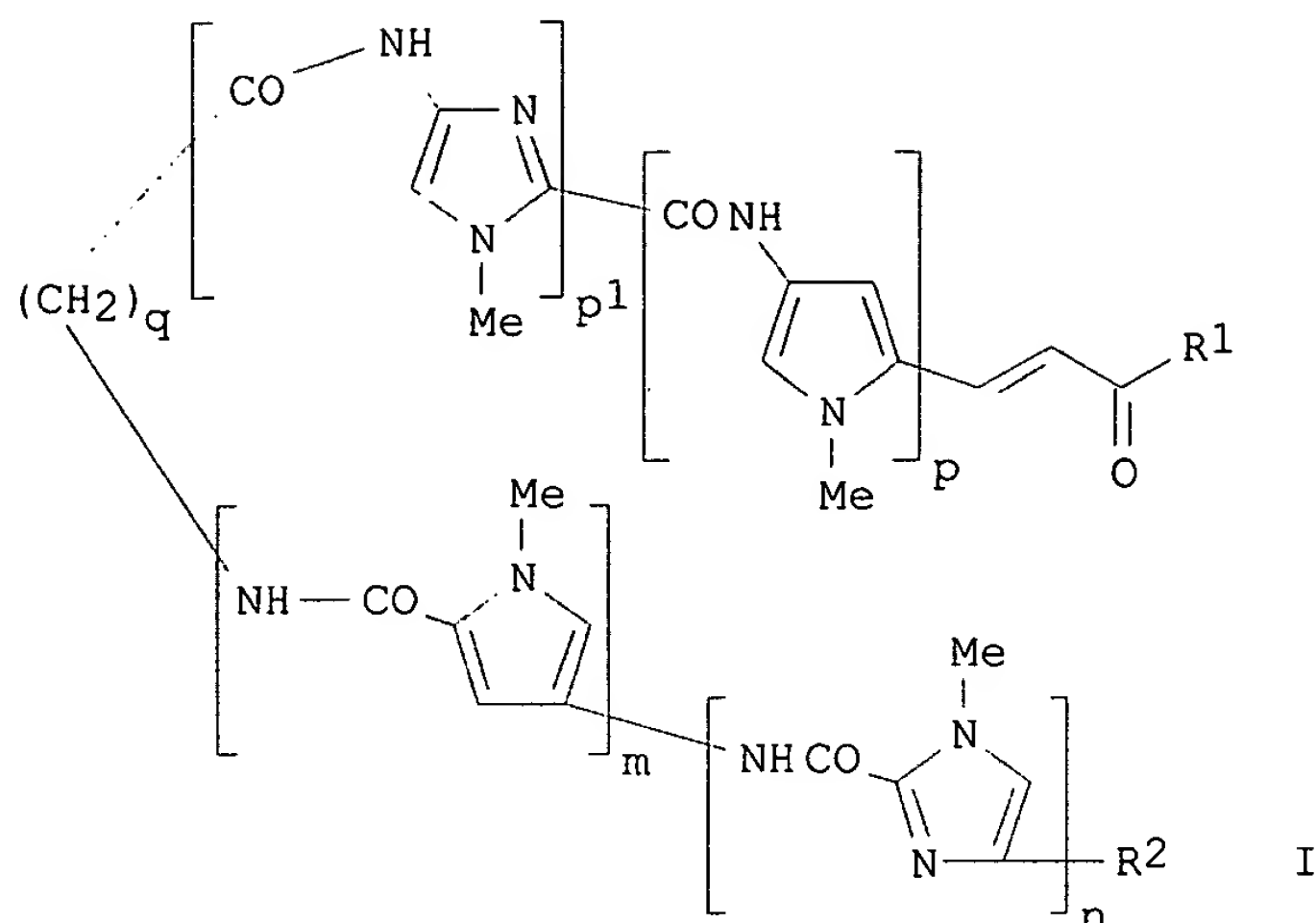
STEREO ATTRIBUTES: NONE
 L11 30 SEA FILE=REGISTRY SUB=L9 SSS FUL L10
 L12 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L11

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=> d ibib abs hitrn l12 1-14

L12 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2003:737733 HCAPLUS
 DOCUMENT NUMBER: 139:276894
 TITLE: Preparation of hairpin-type pyrrole-imidazole
 polyamides as anticancer agents
 INVENTOR(S): Sugiyama, Hiroshi; Bando, Toshikazu; Saito, Isao
 PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan
 SOURCE: PCT Int. Appl., 46 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003076412	A1	20030918	WO 2003-JP2423	20030303
W: US				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
JP 2003261541	A2	20030919	JP 2002-63608	20020308
PRIORITY APPLN. INFO.:			JP 2002-63608	A 20020308
OTHER SOURCE(S):		MARPAT 139:276894		
GI				



AB It is intended to provide a pyrrole-imidazole polyamide type functional mol. having enhanced abilities of alkylating DNA and recognizing a sequence, compared with the existing functional mols. of this type, for a specific base sequence occurring on DNA. Hairpin polyamides have an alkylation site via a vinyl linker at the end of a pyrrole-imidazole polyamide and are represented by general formula (I; R1 = a site for alkylation reaction; R2 = H, alkyl, acetamido; p, p1, q, m, n = an integer). Disclosed are drugs for inhibiting the expression of a specific gene and anticancer agents contg. the above hairpin polyamide. For example, I (m = p = p1 = 1, n = 2, q = 3, R1 = q) selectively alkylated A of the GTCA sequence of DNA (pUC-I'). The compds. I were tested for inhibiting the proliferation of various cancer cells.

IT 491647-63-3P 491647-64-4P 602308-98-5P
602308-99-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of hairpin-type pyrrole-imidazole polyamides for alkylating DNA and inhibiting gene expression as anticancer agents)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:393696 HCAPLUS

DOCUMENT NUMBER: 139:358146

TITLE: Specific alkylation of human telomere repeats by hairpin pyrrole-imidazole polyamide

AUTHOR(S): Takahashi, Ryoko; Bando, Toshikazu; Sugiyama, Hiroshi

CORPORATE SOURCE: Institute of Biomaterials and Bioengineering, Division of Biofunctional Molecules, Tokyo Medical and Dental University, 2-3-10 Surugadai, Kanda, Chiyoda, Tokyo, 101-0062, Japan

SOURCE: Bioorganic & Medicinal Chemistry (2003), 11(12), 2503-2509

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A novel hairpin polyamide-cyclopropapyrroloindole (CPI) conjugate PyImImIm-.gamma.-PyPyPyLDu86 (conjugate 11), which targets human telomere

repeats d(TTAGGG)n/d(CCCTAA)n, was synthesized. High resolu. denaturing PAGE using 44 bp DNA fragments and HPLC product anal. of a synthetic nonanucleotide demonstrated that conjugate 11 alkylates the target adenine in the telomere repeats, 5'-CCCTAA-3'. Examn. of the antitumor activity of conjugate 11 using a panel of 39 cancer cell lines demonstrated that the av. concn. of conjugate 11 required for 50% growth inhibition was 5.75 .mu.M, which is superior to pepleomycin and bleomycin and comparable to cisplatin.

IT 619212-51-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(specific alkylation of human telomere repeats by hairpin pyrrole-imidazole polyamide conjugate in cancer cell lines)

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:341959 HCAPLUS

DOCUMENT NUMBER: 139:345455

TITLE: Gene therapy of cancer by using novel alkylating pyrrole-imidazole polyamide

AUTHOR(S): Sugiyama, Hiroshi

CORPORATE SOURCE: Dep. of Biomaterials, Tokyo Medical and Dental University, Japan

SOURCE: Ikagaku Oyo Kenkyu Zaidan Kenkyu Hokoku (2001), Volume Date 2000, 19, 198-202

CODEN: IOKHEP; ISSN: 0914-5117

PUBLISHER: Ikagaku Oyo Kenkyu Zaidan

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB Novel alkylating pyrrole-imidazole polyamide derivs. were design and prepd. for gene therapy of cancer. The antitumor activities of the derivs. against Hela cells were tested.

IT 339984-88-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(gene therapy of cancer by using novel alkylating pyrrole-imidazole polyamides)

IT 339984-91-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(gene therapy of cancer by using novel alkylating pyrrole-imidazole polyamides)

L12 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:155388 HCAPLUS

DOCUMENT NUMBER: 138:333279

TITLE: Highly Efficient Sequence-Specific DNA Interstrand Cross-Linking by Pyrrole/Imidazole CPI Conjugates

AUTHOR(S): Bando, Toshikazu; Narita, Akihiko; Saito, Isao; Sugiyama, Hiroshi

CORPORATE SOURCE: Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan

SOURCE: Journal of the American Chemical Society (2003), 125(12), 3471-3485

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:333279

AB We have developed a novel type of DNA interstrand crosslinking agent by synthesizing dimers of a pyrrole (Py)/imidazole (Im)-diamide-CPI conjugate, ImPyLDu86, connected using seven different linkers. The tetramethylene linker compd. [I], efficiently produces DNA interstrand-cross-links at the nine-base-pair sequence, 5'-PyGGC(T/A)GCCPu-3', only in the presence of a partner triamide, ImImPy. For efficient crosslinking by I with ImImPy, one A.cntdot.T base pair between two recognition sites was required to accommodate the linker region. Elimination of the A.cntdot.T base pair and insertion of an addnl. A.cntdot.T base pair and substitution with a G.cntdot.C base pair significantly reduced the degree of crosslinking. The sequence specificity of the interstrand crosslinking by I was also examd. in the presence of various triamides. The presence of ImImIm slightly reduced the formation of a cross-linked product compared to ImImPy. The mismatch partners, ImPyPy and PyImPy, did not produce an interstrand cross-link product with I, whereas ImPyPy and PyImPy induced efficient alkylation at their matching site with I. The interstrand crosslinking abilities of I were further examd. using denaturing PAGE with 5'-Texas Red-labeled 400- and 67-bp DNA fragments. The sequencing gel anal. of the 400-bp DNA fragment with ImImPy demonstrated that I alkylates several sites on the top and bottom strands, including one interstrand crosslinking match site, 5'-PyGGC(T/A)GCCPu-3'. To obtain direct evidence of interstrand cross-linkages on longer DNA fragments, a simple method using biotin-labeled complementary strands was developed, which produced a band corresponding to the interstrand cross-linked site on both top and bottom strands. Densitometric anal. indicated that the contribution of the interstrand cross-link in the obsd. alkylation bands was approx. 40%. This compd. efficiently cross-linked both strands at the target sequence. The present system consisted of a 1:2 complex of the alkylating agent and its partner ImImPy and caused an interstrand crosslinking in a sequence-specific fashion according to the base-pair recognition rule of Py-Im polyamides.

IT 373362-22-2P 373362-24-4P 373362-26-6P
373362-27-7P 515867-58-0P 515867-60-4P
515867-62-6P

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(crosslinking; sequence-specific DNA interstrand crosslinking by pyrrole/imidazole CPI conjugates)

REFERENCE COUNT: 76 THERE ARE 76 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:954878 HCAPLUS

DOCUMENT NUMBER: 139:30289

TITLE: Regulation of gene expression by sequence-specific alkylating polyamide

AUTHOR(S): Oyoshi, Takanori; Kawakami, Wakana; Bando, Toshikazu; Narita, Akihiko; Sugiyama, Hiroshi

CORPORATE SOURCE: Division of Biofunctional Molecules, Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan

SOURCE: Nucleic Acids Research Supplement (2002), 2(Twenty-ninth Symposium on Nucleic Acids Chemistry), 259-260

CODEN: NARSCE

PUBLISHER: Oxford University Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In order to investigate the inhibition of gene expression by a new type of hairpin polyamide-CPI conjugate 1, its ability to inhibit transcription in cell free system was investigated. Sequence-selective alkylation of

double-stranded DNA by 1 was investigated by denaturing gel electrophoresis using 1000 bp DNA fragment which codes for green fluorescence protein (GFP) under the control of T7 promoter. Anal. of DNA sequence indicated that 1 alkylated predominantly at the site of 5'-AGTCA-3' in coding region of GFP. The transcript by T7 RNA polymerase using the alkylated DNA as a template was analyzed by PAGE. The results clearly indicate that 1 inhibits transcription by alkylation of coding region at a nanomolar concn.

IT 491647-63-3

RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(regulation of gene expression by sequence-specific alkylating polyamide)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:840303 HCAPLUS

DOCUMENT NUMBER: 138:132742

TITLE: Molecular design of a pyrrole - imidazole hairpin polyamides for effective DNA alkylation

AUTHOR(S): Bando, Toshikazu; Narita, Akihiko; Saito, Isao; Sugiyama, Hiroshi

CORPORATE SOURCE: Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering, Tokyo Medical and Dental University, Tokyo, 101-0062, Japan

SOURCE: Chemistry--A European Journal (2002), 8(20), 4781-4790
CODEN: CEUJED; ISSN: 0947-6539

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:132742

AB New hairpin polyamide-CPI (CPI = cyclopropylpyrroloindole) conjugates, compds. 12-14, were synthesized and their DNA-alkylating activities compared with the previously prepd. hairpin polyamide, compd. 1, by high-resoln. denaturing gel electrophoresis with 450 base pair (bp) DNA fragments and by HPLC product anal. of the synthetic decanucleotide. In accord with our previous results, alkylation by compd. 1 occurred predominantly at the G moiety of the sequence 5'-AGTCAG-3' (site 3). However, compd. 12, in which the structure of the alkylating moiety of compd. 1 is replaced with segment A of duocarmycin A DU-86 (CPI), did not show any DNA alkylating activity. In clear contrast, the hairpin CPI conjugate 13, which differs from compd. 1 in that it lacks one Py unit and possesses a vinyl linker, alkylated the A of 5'-AGTCAG-3' (site 3) efficiently at nanomolar concns. Alkylation by compd. 14, which has a vinyl linker, occurred at the A of 5'-AGTCCA-3' (site 6) and at several minor alkylation sites, including mismatch alkylation at A of 5'-TCACAA-3' (site 2). The significantly different reactivity of the alkylating hairpin polyamides 1, 12, 13, and 14 was further confirmed by HPLC product anal. by using a synthetic decanucleotide. The results suggest that hairpin polyamide-CPI conjugate 13 alkylates effectively according to Dervan's pairing rule, and with a new mode of recognition in which the Im-vinyl linker (L) pair targets G-C base pairs. These results demonstrate that incorporation of the vinyl-linker pairing with Im dramatically improves the reactivity of hairpin polyamide-CPI conjugates.

IT 491647-63-3P 491647-64-4P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(vinyl-linker pairing with imidazole in pyrrole - imidazole hairpin can improve polyamides for effective DNA alkylation)

REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:666652 HCAPLUS
DOCUMENT NUMBER: 138:85083
TITLE: Sequence-specific protection of plasmid DNA from
restriction endonuclease hydrolysis by
pyrrole-imidazole-cyclopropapyrroloindole conjugates
AUTHOR(S): Fujimoto, Kazuhisa; Iida, Hirokazu; Kawakami, Masako;
Bando, Toshikazu; Tao, Zhi-Fu; Sugiyama, Hiroshi
CORPORATE SOURCE: Institute of Biomaterials and Bioengineering, Division
of Biofunctional Molecules, Tokyo Medical and Dental
University, Chiyoda, Tokyo, 101-0062, Japan
SOURCE: Nucleic Acids Research (2002), 30(17), 3748-3753 -
CODEN: NARHAD; ISSN: 0305-1048
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The pyrrole-imidazole (Py-Im) triamide-cyclopropa pyrroloindole (CPI)
conjugates ImPyImLDu86 (7) and ImImPyLDu86 (14) were synthesized and their
alkylating activities and inhibitory effects on DNA hydrolysis by
restriction endonucleases were examd. Sequencing gel anal. demonstrated
that conjugates 7 and 14 specifically alkylated DNA at 5'-CGCGCG-3' and
5'-PyGGCCPu-3', resp. Agarose gel electrophoresis indicated that
incubation of a supercoiled plasmid, pSPORT I (4109 bp), with conjugate 7
effectively inhibited its hydrolysis by BssHII (5'-GCGCGC-3'), whereas
conjugate 14 had no effect on this hydrolysis. These results suggest that
conjugate 7 sequence-specifically inhibits the hydrolysis of DNA by
BssHII. Sequence-specific alkylation by the Py-Im triamide-CPI conjugates
was further confirmed by inhibition of the Eco52I (5'-CGGCCG-3')
hydrolysis of conjugate 14-treated pQBI PGK (5387 bp). In clear contrast,
hydrolysis of pQBI PGK by DraI (3'-TTTAAA-3') was not inhibited by 5 .mu.M
conjugate 14. That ImImPy did not inhibit the hydrolysis of pQBI PGK
indicates that covalent bond formation is necessary for inhibition. A
similar expt., using linear pQBI PGK, achieved the same extent of
protection of the DNA with approx. half the concn. of conjugate 14 as was
required to protect supercoiled DNA from hydrolysis.

IT 484017-85-8P 484017-86-9P

RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);
BIOL (Biological study); PREP (Preparation)
(sequence-specific protection of plasmid DNA from restriction
endonuclease hydrolysis by pyrrole-imidazole-cyclopropapyrroloindole
conjugates)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:833321 HCAPLUS
DOCUMENT NUMBER: 135:371743
TITLE: Preparation of pyrrole-imidazole polyamide-duocarmycin
segment conjugates as interstrand crosslinking agents
for DNA in cancer treatment
INVENTOR(S): Sugiyama, Hiroshi; Bando, Toshikazu; Iida, Hirokazu;
Saito, Isao
PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001085733	A1	20011115	WO 2001-JP3756	20010501

W: US
 RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
 PT, SE, TR
 JP 2001322992 A2 20011120 JP 2000-140361 20000512
 EP 1281711 A1 20030205 EP 2001-926081 20010501
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
 IE, FI, CY, TR
 PRIORITY APPLN. INFO.: JP 2000-140361 A 20000512
 WO 2001-JP3756 W 20010501
 OTHER SOURCE(S): MARPAT 135:371743
 GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Compds. represented by the following general formula A-L-B-X-B-L-A (I; wherein B represents a chem. structure capable of recognizing a base sequence of a DNA; A represents a chem. structure capable of binding to one of the bases of the DNA; L represents a linker by which the chem. structures A and B can be linked to each other; and X represents a spacer by which the A-L-B components can be linked to each other), by which two DNA strands can be interstrand-crosslinked, are prepd. Also claimed are a method of interstrand-crosslinking DNA by using these compds. and medicinal compns. contg. interstrand crosslinking agents of DNA. In the compds. I, the above chem. structure capable of recognizing a base sequence of a DNA is derived from pyrrole and/or imidazole and the chem. structure capable of binding to one of the bases of the DNA possesses a cyclopropane ring. More specifically, the compds. represented by N-[3-[4-(N-methylimidazol-2-ylcarbonylamino)-N-methylpyrrol-2-yl]acryloyl]cyclopropa[c]pyrrolo[3,2-e]indole derivs. (pyrrole-imidazole polyamide-duocarmycin segment conjugates) [II; X = CO, COCH:CHCO, CO(CH₂)₄CO, CO-p-C₆H₄-CO] are prepd. The B component in the compds. I, i.e. the 4-(N-methylimidazol-2-ylcarbonylamino)-N-methylpyrrole moiety of II, recognizes a DNA base sequence and is capable of specifically interstrand-crosslinking to the specific base sequence of DNA. These compds. inhibit the replication of DNA by interstrand-crosslinking to DNA and thereby are useful for the treatment of cancer. Interstrand-crosslinking reaction of the compds. II to DNA oligomers was examd. using polyacrylamide gel electrophoresis. For example, it was confirmed that II [X = CO(CH₂)₄CO] interstrand-crosslinked to the TGGC or GCCA or its complimentary sequence of DNA, in particular in the copresence of a triamide (III; X = Y = N and Z = CH; X = Y = Z = N; X = N and Y = Z = CH; X = Z = CH and Y = N).

IT 373362-22-2P 373362-24-4P 373362-26-6P
 373362-27-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (prepn. of pyrrole-imidazole polyamide-duocarmycin conjugates as DNA interstrand crosslinking agents for treatment of cancer)

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:365880 HCAPLUS

DOCUMENT NUMBER: 134:366795

TITLE: DNA sequence recognition by pyrrole-imidazole

polyamide for use in anticancer drug screening

INVENTOR(S): Sugiyama, Hiroshi; Saito, Akira; Iida, Hirokazu

PATENT ASSIGNEE(S): Foundation for Scientific Technology Promotion, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

DOCUMENT TYPE: CODEN: JKXXAF
 LANGUAGE: Patent
 FAMILY ACC. NUM. COUNT: 1 Japanese
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001136974	A2	20010522	JP 1999-326007	19991116
WO 2001036677	A1	20010525	WO 2000-JP7992	20001113
W: US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
EP 1152061	A1	20011107	EP 2000-974961	20001113
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 2003099998	A1	20030529	US 2002-285030	20021101
PRIORITY APPLN. INFO.:			JP 1999-326007	A 19991116
			WO 2000-JP7992	W 20001113
			US 2001-889379	A3 20010716

AB Novel chem. species represented by the following general formula B-L-A (B = a chem. structure capable of recognizing the base sequence of DNA, for example, optionally substituted pyrrole-imidazole polyamide; A = a chem. structure capable of binding to unnatural nucleotide bases, for example, the alkylation moiety of duocarmycin A; L = a linker capable of binding the chem. structures A and B, for example, vinyl) and use of those compds. in screening of biol. activity of chem. compds. are disclosed. Those compds. are preferably DNA alkylating agents, applicable as anticancer agents. Reagent kits for screening, including microtiter plates, are claimed. Drug screening using human cancer cell lines, CL-wt cells, HLC-2 cells, Jurkat cells, and HeLa cells, and synthetic scheme for the bioactive compds., are described.

IT **339984-88-2 339984-91-7**
 RL: ARU (Analytical role, unclassified); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); ANST (Analytical study); BIOL (Biological study); PROC (Process); USES (Uses)
 (DNA sequence recognition by pyrrole-imidazole polyamide for use in anticancer drug screening)

IT **339984-92-8P**
 RL: ARU (Analytical role, unclassified); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
 (DNA sequence recognition by pyrrole-imidazole polyamide for use in anticancer drug screening)

L12 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN
 ACCESSION NUMBER: 2001:327062 HCAPLUS
 DOCUMENT NUMBER: 135:102536
 TITLE: Sequence-specific DNA interstrand cross-linking by imidazole-pyrrole CPI conjugate
 AUTHOR(S): Bando, Toshikazu; Iida, Hirokazu; Saito, Isao; Sugiyama, Hiroshi
 CORPORATE SOURCE: CREST Japan Science and Technology Corporation (JST) Japan Division of Biofunctional Molecules Institute of Biomaterials and Bioengineering Tokyo Medical and Dental University, Kanda Chiyoda Tokyo, 101-0062, Japan
 SOURCE: Journal of the American Chemical Society (2001), 123(21), 5158-5159

CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB DNA interstrand crosslinking inhibits both DNA replication and gene expression and therefore has considerable potential for mol. biol. and human medicine. However, an interstrand crosslinking agent that targets a predetd. base-pair sequence has not been achieved. Minor-groove binding polyamides that contain N-methylimidazole (Im)-N-methylpyrrole (Py)hydroxypyrrole (Hp), which uniquely recognize each of the four Watson-Crick base pairs, can be used as novel recognition parts of sequence-specific DNA alkylating agents. We also demonstrated that Im7Py diamide-CPI conjugate with a vinyl linker, ImPyLDu86, alkylates double-stranded DNA at predetd. sequences through highly cooperative homodimer formation. Herein we describe the synthesis of a covalent dimer of ImPyLDu86 connected with various linkers and their DNA interstrand crosslinking abilities. In conclusion, we developed a novel DNA interstrand crosslinking agent, that crosslinked double strands only in the presence of ImImPy at a nine-base-pair sequence, 5'-PyGGC(T/A)GCCPu-3'. The present system will provide a promising approach for the design of novel sequence-specific DNA interstrand crosslinking agents. Targeting specific sequences in the human genome by such sequence-specific crosslinking agent would constitute a powerful gene-regulating tool. Further studies on the applicability of this novel class of crosslinking agents are currently in progress.

IT 349647-78-5 349647-79-6 349647-80-9
 349647-82-1 349647-83-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
 (sequence-specific DNA interstrand crosslinking by imidazole-pyrrole CPI conjugate)

IT 349647-81-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (sequence-specific DNA interstrand crosslinking by imidazole-pyrrole CPI conjugate)

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:707167 HCAPLUS

DOCUMENT NUMBER: 133:266852

TITLE: Preparation of duocarmycin derivatives capable of cleaving double-stranded DNA and method of utilization of the same

INVENTOR(S): Sugiyama, Hiroshi; Tao, Zhi-Fu; Saito, Isao

PATENT ASSIGNEE(S): Japan Science and Technology Corporation, Japan

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000058312	A1	20001005	WO 2000-JP1461	20000310
W: CA, KR, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 2000281679	A2	20001010	JP 1999-83591	19990326
CA 2328903	AA	20001005	CA 2000-2328903	20000310

EP 1083177 A1 20010314 EP 2000-907992 20000310

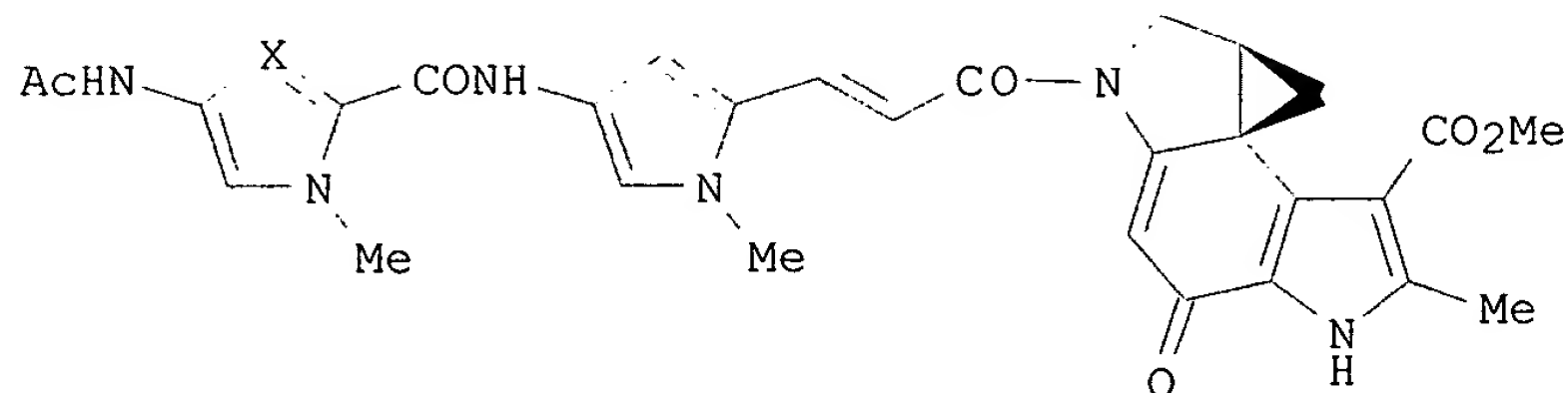
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, FI

PRIORITY APPLN. INFO.:

JP 1999-83591 A 19990326

WO 2000-JP1461 W 20000310

GI



AB Novel chem. species represented by the following general formula B-L-A (I; wherein B represents a chem. structure capable of recognizing the base sequence of DNA, for example, optionally substituted pyrrole-imidazole polyamide; A represents a chem. structure capable of binding to one base of DNA, for example, the alkylation moiety of duocarmycin A; and L represents a linker capable of binding the chem. structures A and B, for example, vinyl) are prepd. Also claimed are a method for alkylating DNA and a method for cleaving double-stranded DNA by using these compds.; and medicinal compns. with the use of these compds. for treatment of cancer. These compds. I, e.g. duocarmycin derivs. (II; R = CH, N) (prepn. given) which recognizes base sequences TGACG or CGACG or their complimentary chain, are capable of simultaneously alkylating double-stranded DNA and cleaving the same and useful as artificial restriction enzymes or for targeting specific DNA base sequences for gene therapy. II (R = CH), II (R = N), and duocarmycin A in vitro showed IC₅₀ of 1.5, 0.7 nM, and 4.7, resp., for inhibiting the proliferation of HeLaS3 cells.

IT 296794-37-1P 296794-38-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of duocarmycin derivs. capable of alkylating and cleaving double-stranded DNA as anticancer agents)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:96276 HCAPLUS

DOCUMENT NUMBER: 132:275556

TITLE: Highly cooperative DNA dialkylation by the homodimer of imidazole-pyrrole diamide-CPI conjugate with vinyl linker

AUTHOR(S): Tao, Zhi-Fu; Saito, Isao; Sugiyama, Hiroshi

CORPORATE SOURCE: CREST, Japan Science and Technology Corporation (JST), Japan

SOURCE: Journal of the American Chemical Society (2000), 122(8), 1602-1608

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:275556

AB We synthesized new type of diamide-CPI conjugate possessing a vinyl linker (7). Sequence-selective alkylation of double-stranded DNA by 7 was investigated by high-resoln. denaturing gel electrophoresis using

.apprx.400 bp DNA fragments. Highly efficient alkylation predominantly occurs simultaneously at the purines of 5'-PyG(A/T)CPu-3' site on both strands at a nanomolar concn. of 7. These results suggest that the homodimer of conjugate 7 dialkylates both strands according to Dervan's pairing rule together with a new mode of recognition in which the Im-vinyl linker (L) pair targets G/C base pairs. In addn. to the major dialkylation sites, a minor alkylation site was also obsd. at 5'-GT(A/T)GC-3'. This alkylation can be explained by an analogous slipped homodimer recognition mode in which the L-L pair recognizes the A/T base pair. Efficient dialkylation by the homodimer of 7 was further confirmed using oligonucleotides (ODNs). HPLC anal. revealed that the conjugate 7 simultaneously alkylates GN3/AN3 of the target sequences on both strands of ODNs.

IT 263710-69-6P

RL: NUU (Other use, unclassified); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. and cooperative DNA dialkylation by imidazole-pyrrole diamide-CPI conjugate with vinyl linker)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:674932 HCAPLUS

DOCUMENT NUMBER: 132:22791

TITLE: Synthesis and antitumor activity of duocarmycin derivatives: a-ring pyrrole compounds bearing 5-membered heteroarylacryloyl groups

AUTHOR(S): Amishiro, Nobuyoshi; Nagamura, Satoru; Kobayashi, Eiji; Okamoto, Akihiko; Gomi, Katsushige; Saito, Hiromitsu

CORPORATE SOURCE: Pharmaceutical Research Institute, Kyowa Hakko Kogyo Company, Ltd., Shizuoka, 411-8731, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1999), 47(10), 1393-1403

CODEN: CPBTAL; ISSN: 0009-2363

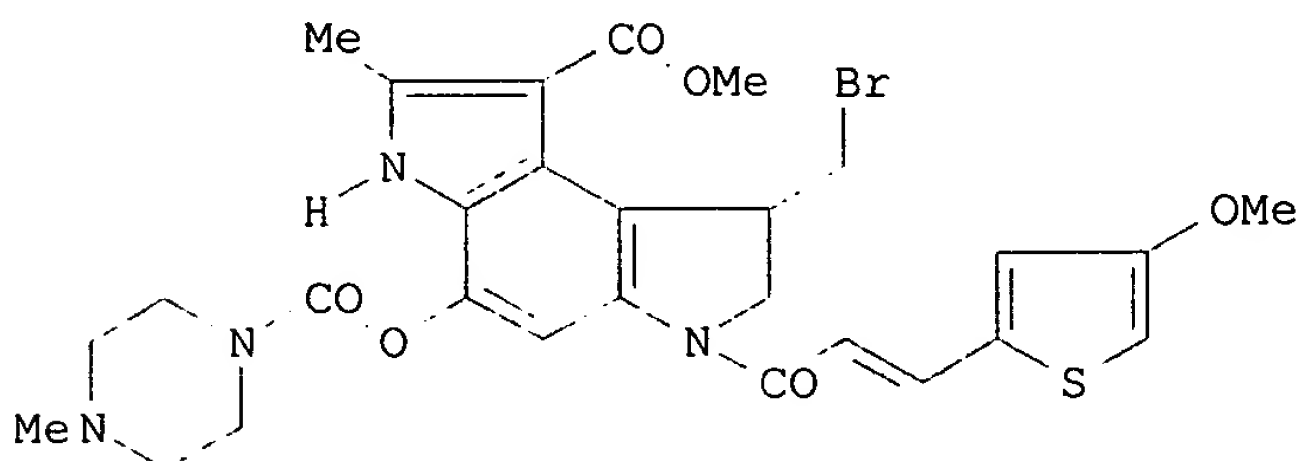
PUBLISHER: Pharmaceutical Society of Japan

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:22791

GI



I

AB A series of A-ring pyrrole compds. of duocarmycin bearing 5-membered heteroarylacryloyl groups (thienylacryloyl and pyrrolylacryloyl) and heteroarylcarbonyl groups were synthesized and evaluated for in vitro anticellular activity against HeLa S3 cells and in vivo antitumor activity against murine sarcoma 180 in mice. Most of the thienylacrylates displayed in vitro anticellular activity equiv. to 4'-methoxycinnamates. Among the 8-O-[(N-methylpiperazinyl)carbonyl] derivs. of

methoxy-thienylacrylates, compd. I, having 4'-methoxy-2'-thienylacryloyl as segment-B (Seg-B), showed remarkably potent antitumor activity and low peripheral blood toxicity in vivo, which were equal to those of 8-O-[(N-methylpiperazinyl)carbonyl] derivs. of 4'-methoxycinnamates, compared with the A-ring pyrrole derivs. having the trimethoxyindole skeleton in Seg-B. On the other hand, the 2'-pyrrolylacrylates having a double bond as spacer showed 102- to 103-fold stronger anticellular activity than 2'-pyrrolecarboxylates (IC₅₀<0.3 nM, 72h-exposure). The 8-O-acetate and 8-O-[(N-methylpiperazinyl)carbonyl] derivs. of 2'-pyrrolylacrylates exhibited an antitumor effect at a lower dose compared with the 8-O-[(N-methylpiperazinyl)carbonyl] derivs. with a 4'-methoxycinnamoyl moiety. Moreover, it was expected that the antitumor activity would be increased by the strength of the extra hydrogen bond formed between the nitrogen of the pyrrole amido group and DNA, owing to the increase of the no. of N-methyl-2'-pyrrolecarboxamide units. However, 2'-pyrrolylacrylates having three N-methyl-2'-pyrrolecarboxamide units showed nearly equal antitumor activity to 2'-pyrrolylacrylates having only one N-methyl-2'-pyrrolecarboxamide unit.

IT 251999-80-1P 251999-81-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(synthesis and antitumor activity of duocarmycin derivs. bearing 5-membered heteroarylacryloyl groups)

REFERENCE COUNT: 74 THERE ARE 74 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:87732 HCAPLUS

DOCUMENT NUMBER: 128:154100

TITLE: Preparation of DC-89 derivatives as antitumor agents

INVENTOR(S): Amishiro, Nobuyoshi; Saito, Hiromitsu; Okamoto, Akihiko; Gomi, Katsushige; Okabe, Masami

PATENT ASSIGNEE(S): Kyowa Hakko Kogyo Co., Ltd., Japan; Amishiro, Nobuyoshi; Saito, Hiromitsu; Okamoto, Akihiko; Gomi, Katsushige; Okabe, Masami

SOURCE: PCT Int. Appl., 57 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9803509	A1	19980129	WO 1997-JP2516	19970722
W: AU, BG, BR, CA, CN, CZ, HU, JP, KR, MX, NO, NZ, PL, RO, SG, SI, SK, UA, US, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9734631	A1	19980210	AU 1997-34631	19970722
PRIORITY APPLN. INFO.:			JP 1996-192634	19960723
			WO 1997-JP2516	19970722

OTHER SOURCE(S): MARPAT 128:154100

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. (I) wherein (II) represents (III) or (IV) [X = Cl, Br; R = H, COR₁, etc.; R₁ = H, (un)substituted alkyl, etc.], and W represents (V) or (VI) (Y₁, Y₂ = O, S, etc.; Q₁-Q₅ = H, alkoxy, NO₂, etc.; m = 0-1; n

= 0-2), are prepd. I are useful as antitumor agents. Compd. (VII) was treated with NaH and then reacted with compd. (VIII) to give 73% the title compd. (IX), which showed IC50 of 2.9 nM against HeLaS3 cell.

IT 202419-12-3P 202419-15-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of DC-89 derivs. as antitumor agents)

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> fil caold

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FILE COVERS 1907-1966

FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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L13 0 L11

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=> fil reg

FILE 'REGISTRY' ENTERED AT 17:56:23 ON 31 JAN 2004

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 JAN 2004 HIGHEST RN 644468-14-4

DICTIONARY FILE UPDATES: 30 JAN 2004 HIGHEST RN 644468-14-4

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

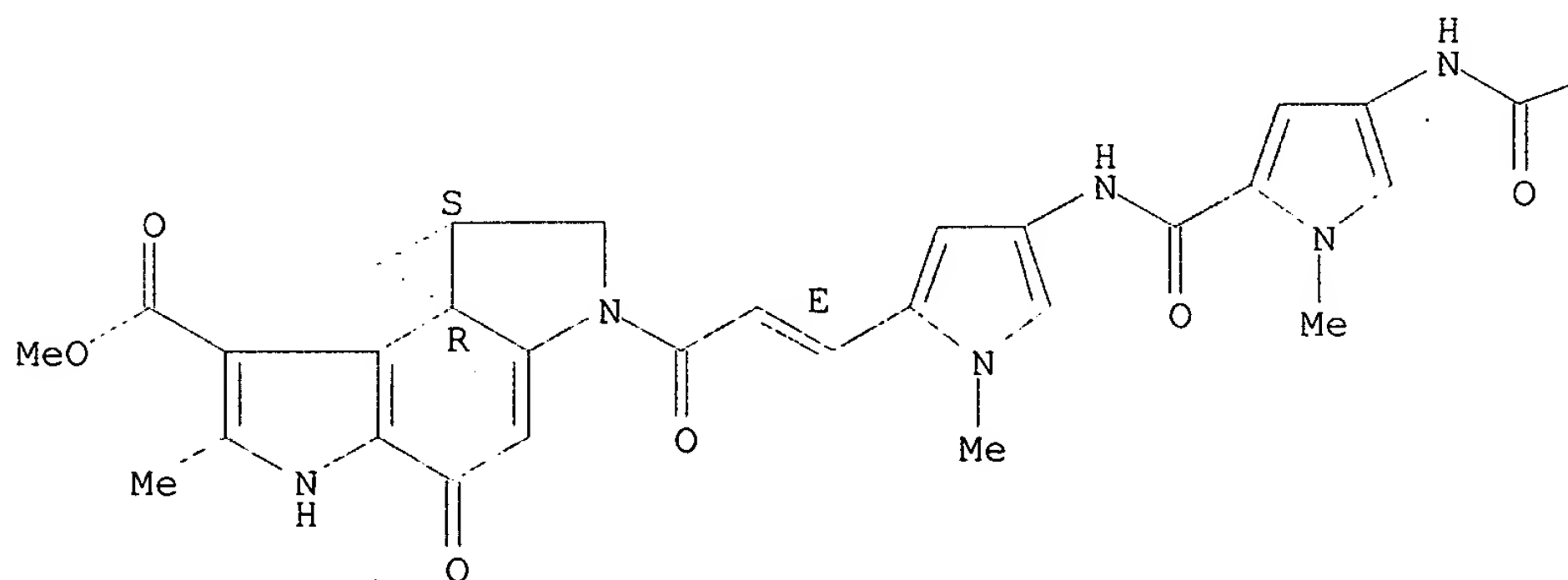
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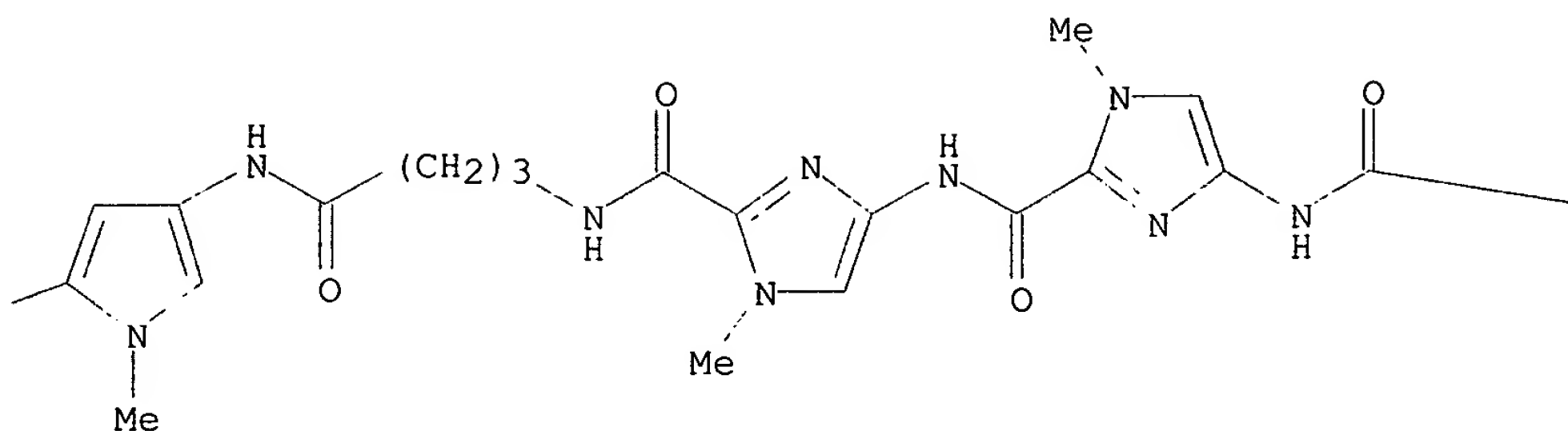
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 LC STN Files: CA, CAPLUS, TOXCENTER

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 Double bond geometry as shown.

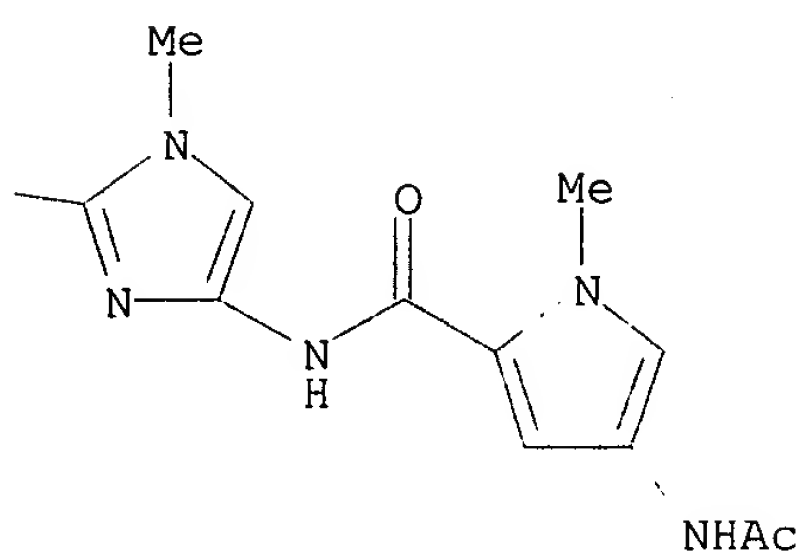
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PAGE 1-B



PAGE 1-C



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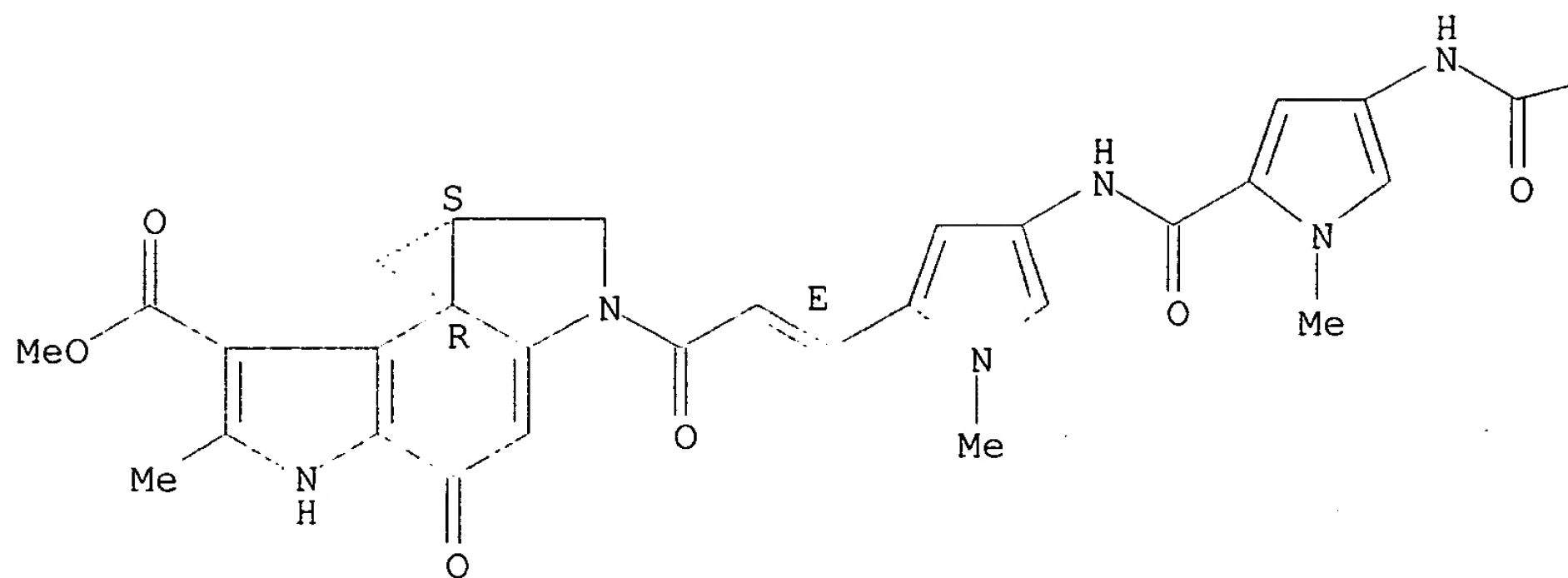
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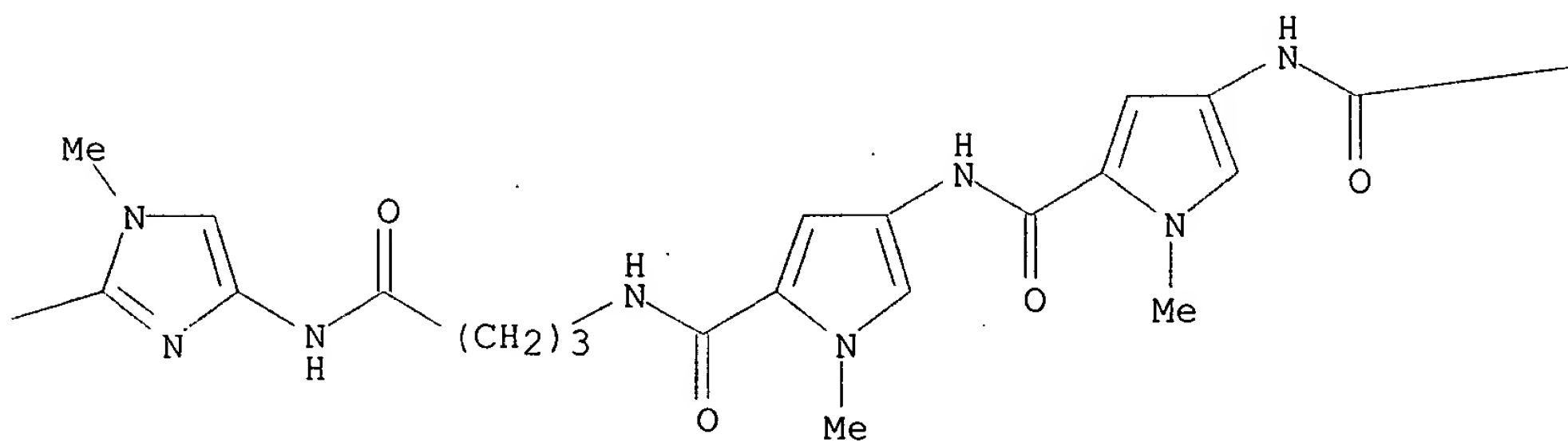
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     imidazol-2-yl]carbonyl]amino]-1H-pyrrol-2-yl]carbonyl]amino]-1H-pyrrol-2-
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LC   STN Files:    CA, CAPLUS, TOXCENTER
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Absolute stereochemistry.
Double bond geometry as shown.

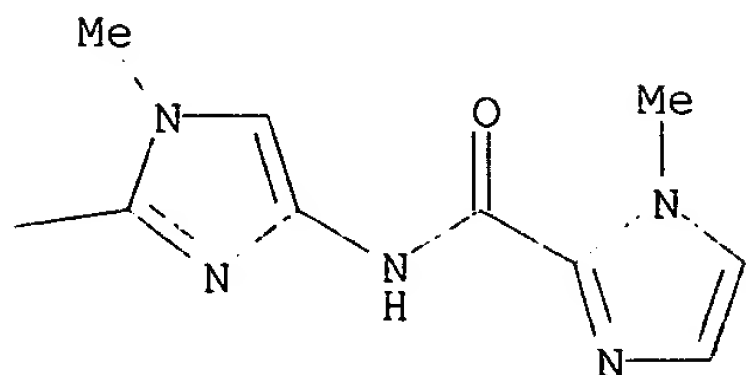
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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:276894

L11 ANSWER 3 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 602308-98-5 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI)
(CA INDEX NAME)

FS STEREOSEARCH

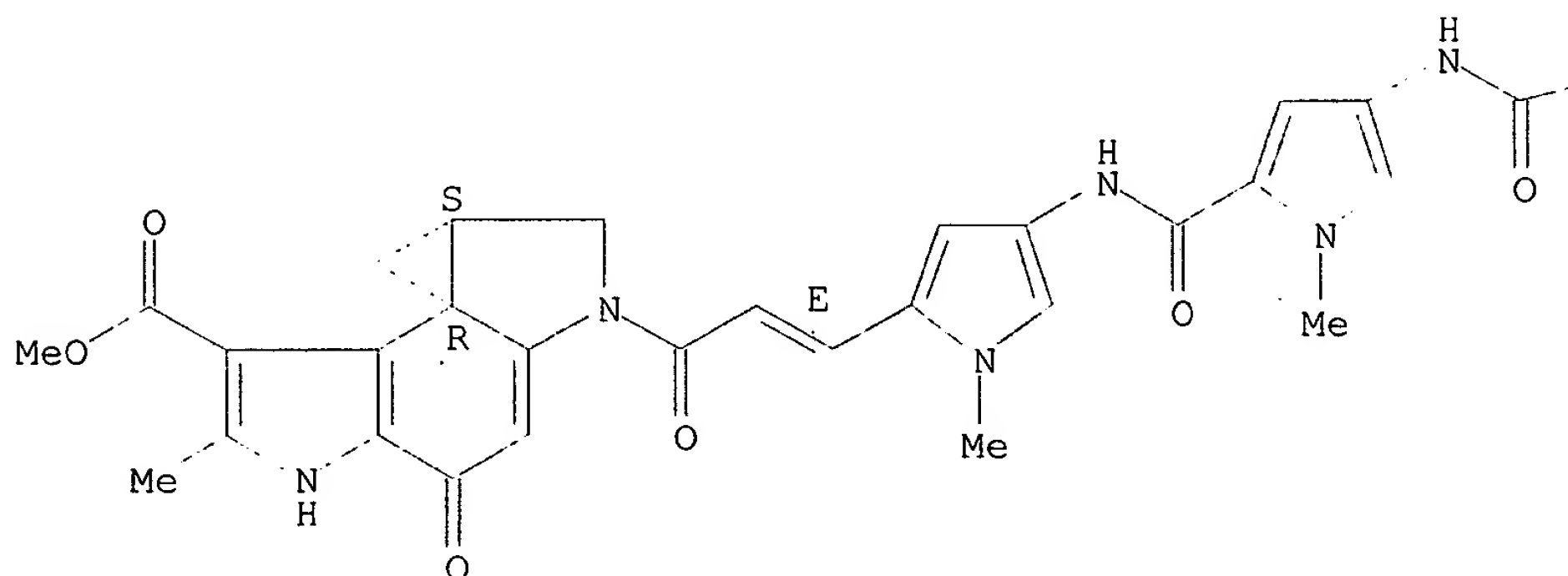
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SR CA

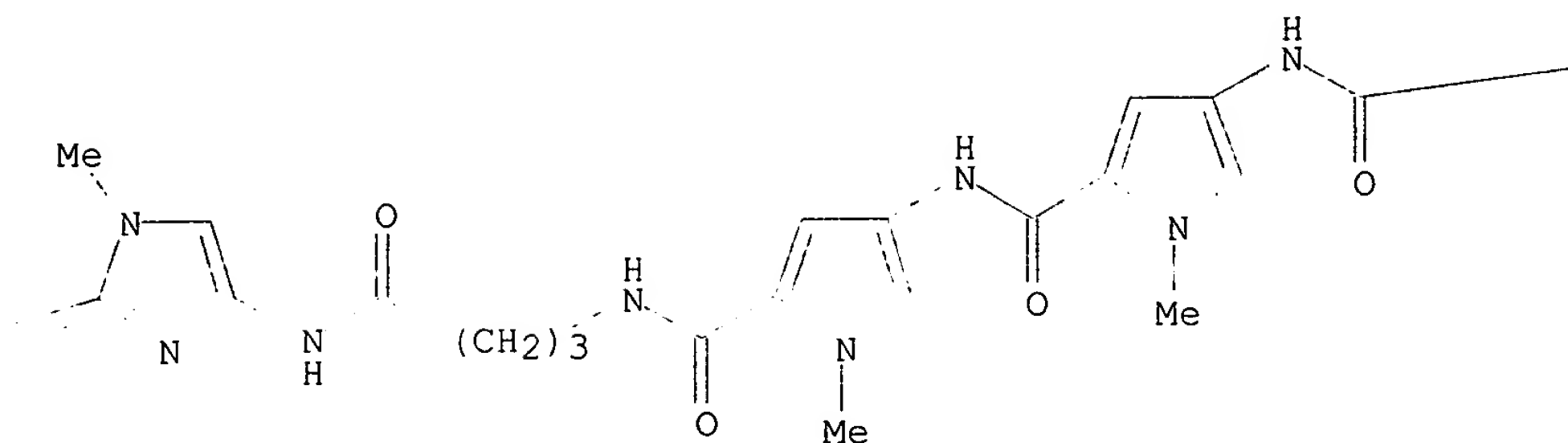
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

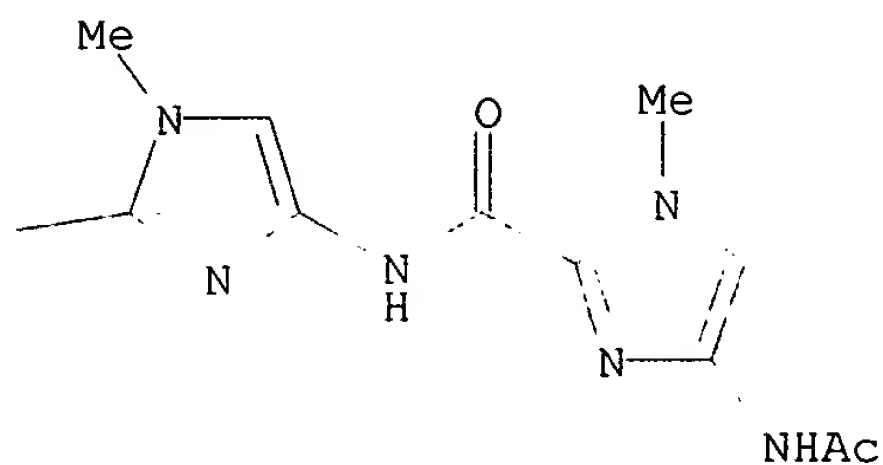
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PAGE 1-C



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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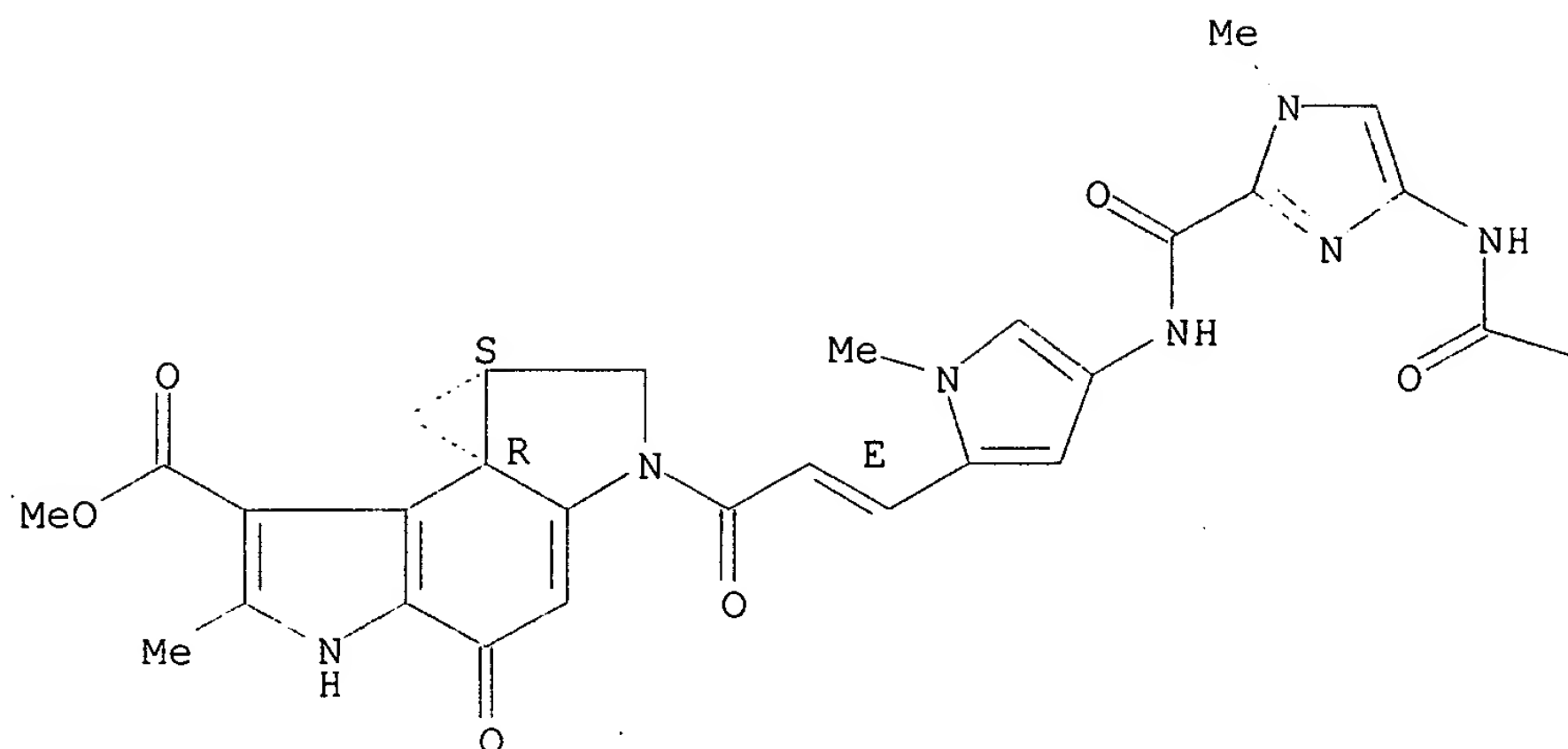
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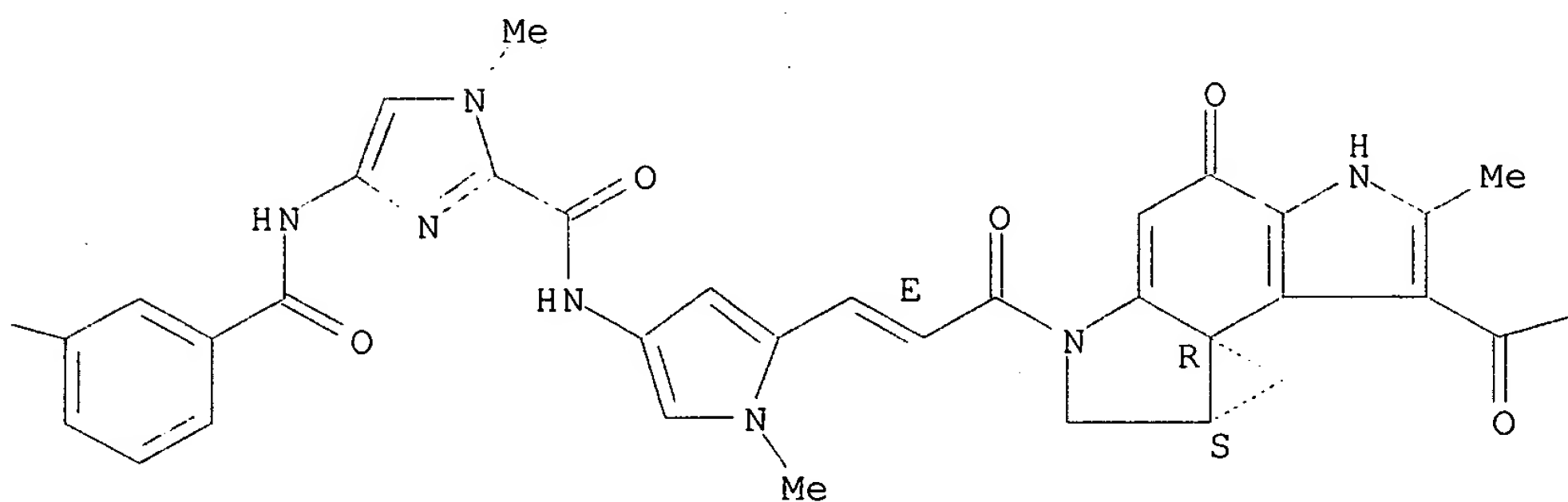
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 RN 515867-62-6 REGISTRY
 CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,3-phenylenebis(carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl))[(2E)-1-oxo-2-propene-3,1-diyl]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C62 H56 N14 O12
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
 Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PAGE 1-C

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

X REFERENCE 1: 138:333279

L11 ANSWER 5 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 515867-60-4 REGISTRY

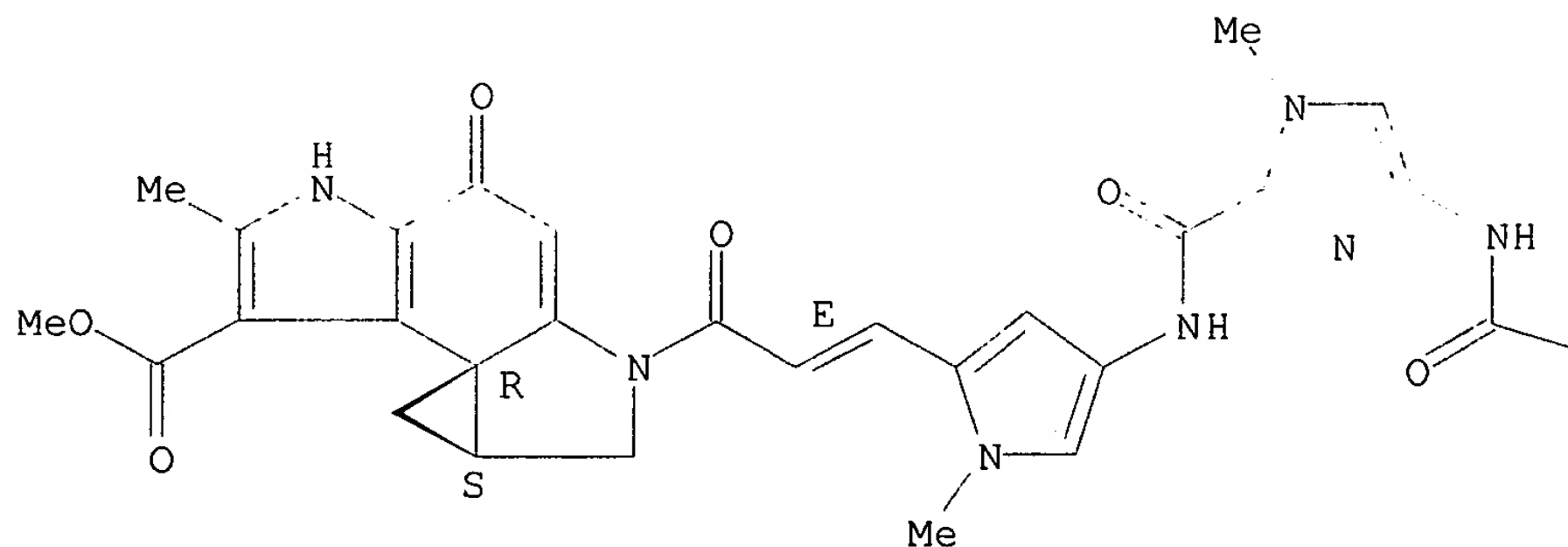
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,7-dioxo-1,7-

heptanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)][(2E)-1-oxo-2-propene-3,1-diyl]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)-(9CI) (CA INDEX NAME)

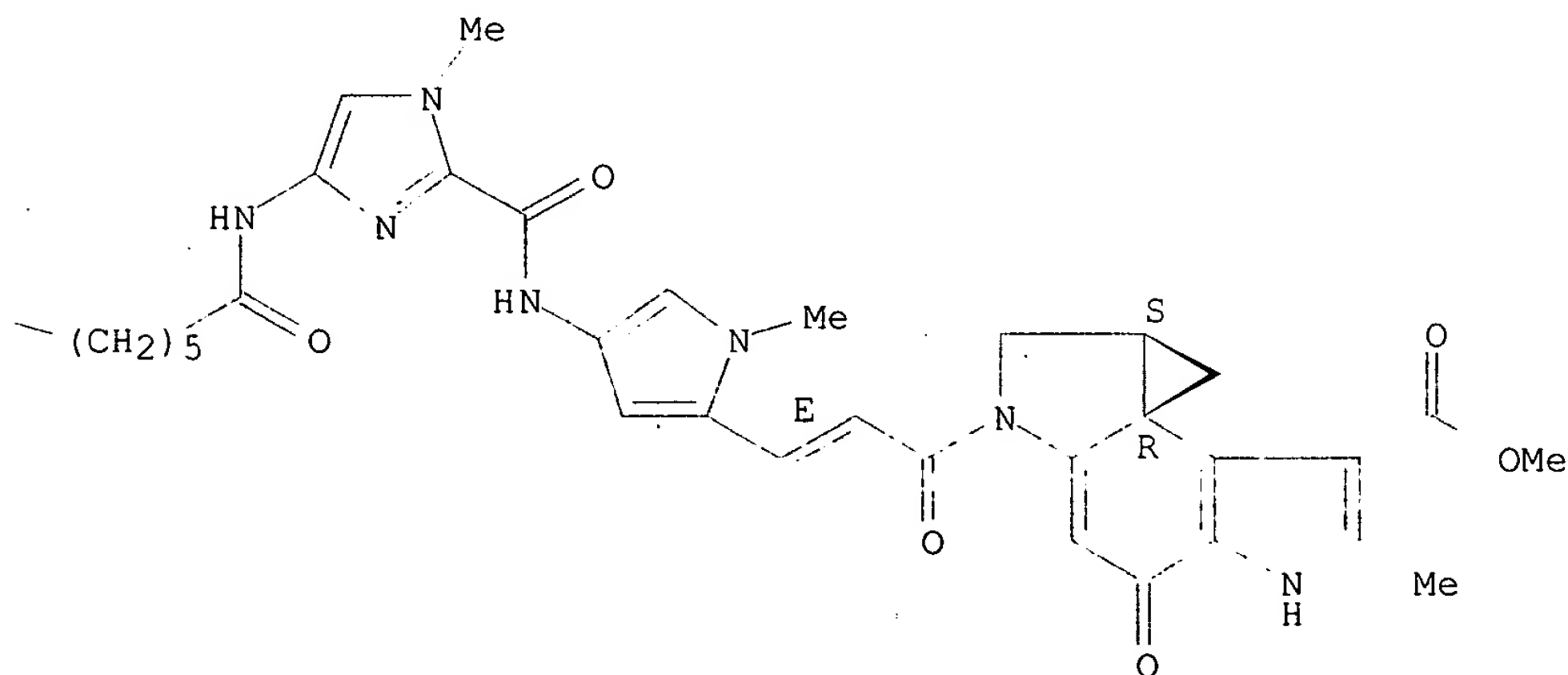
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LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
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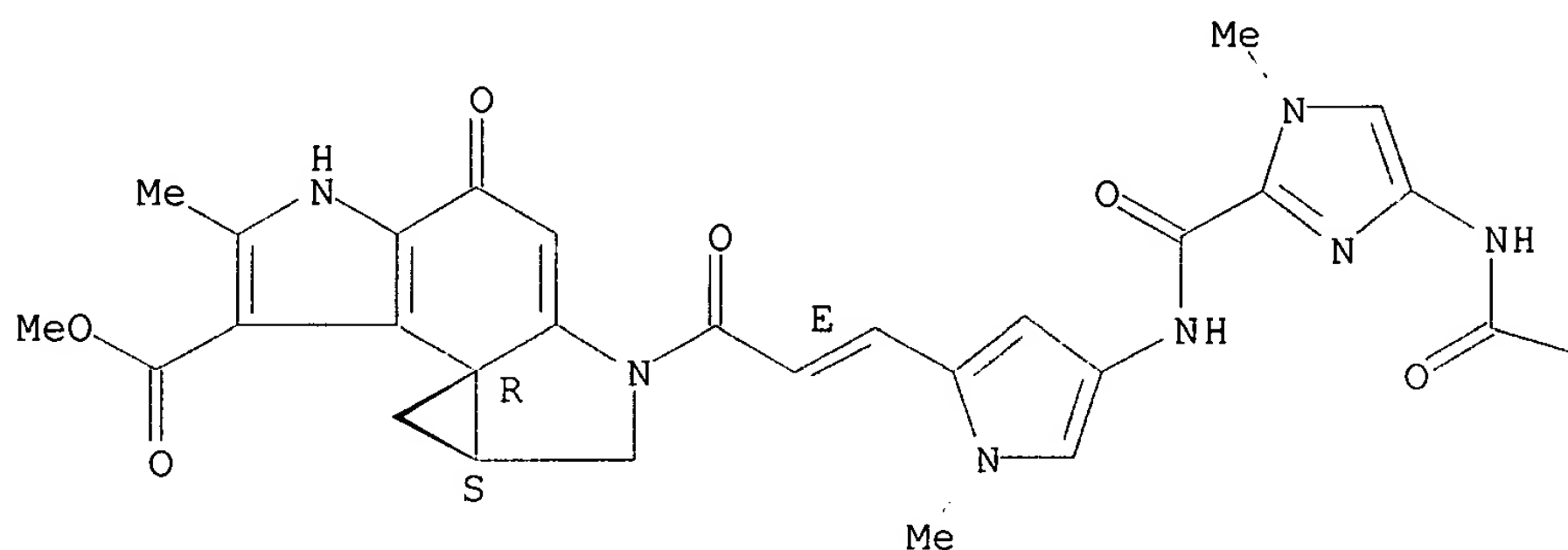
L11 ANSWER 6 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 515867-58-0 REGISTRY
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methyl-1H-pyrrole-4,2-diyl)[(2E)-1-oxo-2-propene-3,1-diyl]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)

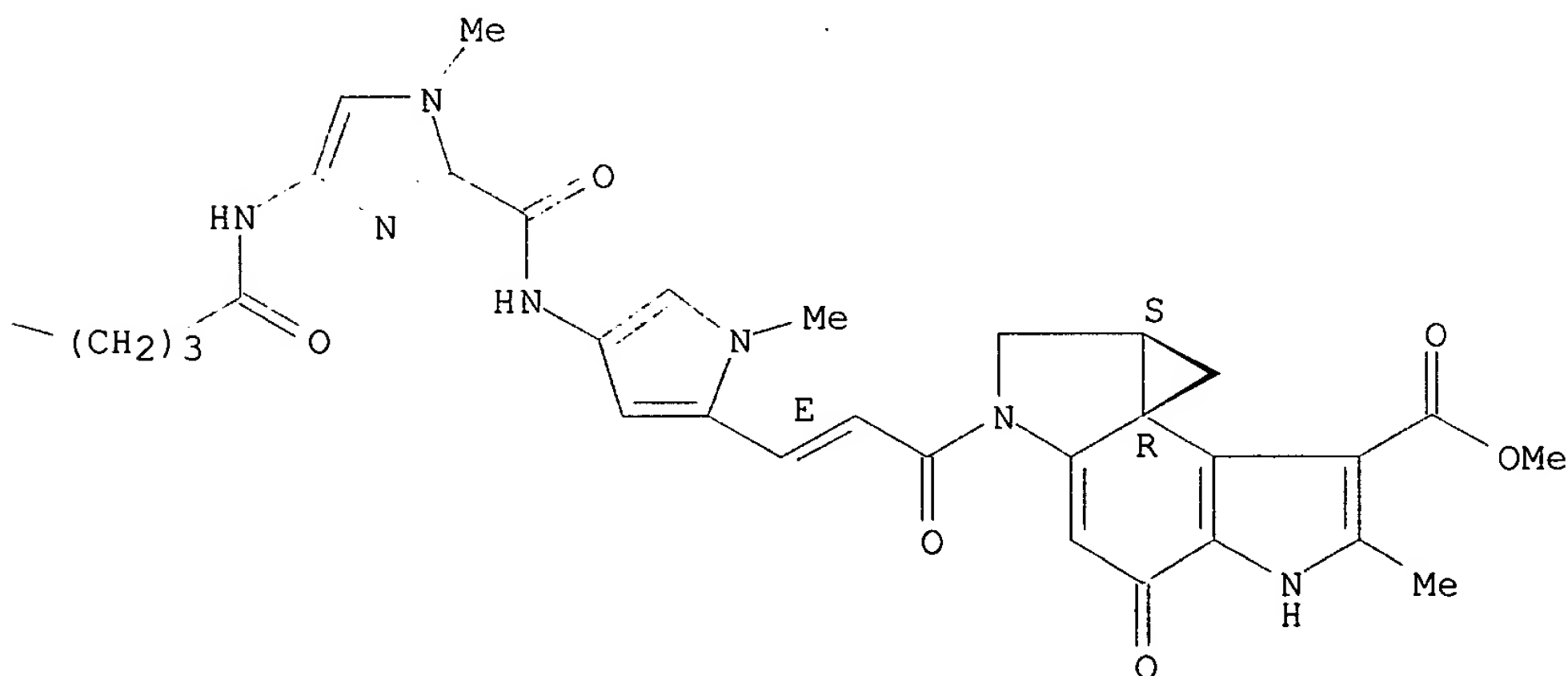
FS STEREOSEARCH
MF C59 H58 N14 O12
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

L11 ANSWER 7 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 491647-64-4 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonylamino]-1-methyl-1H-pyrrol-2-yl]carbonylamino]-1-methyl-1H-

pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C56 H59 N17 O11

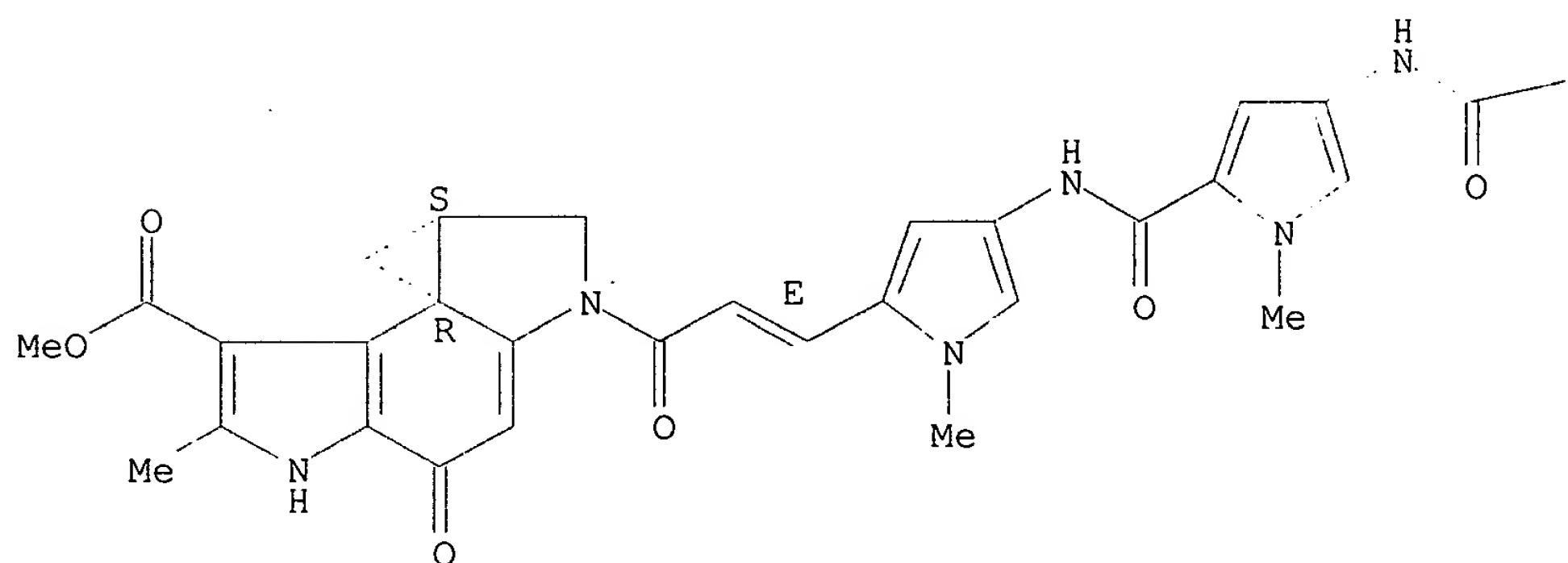
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LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

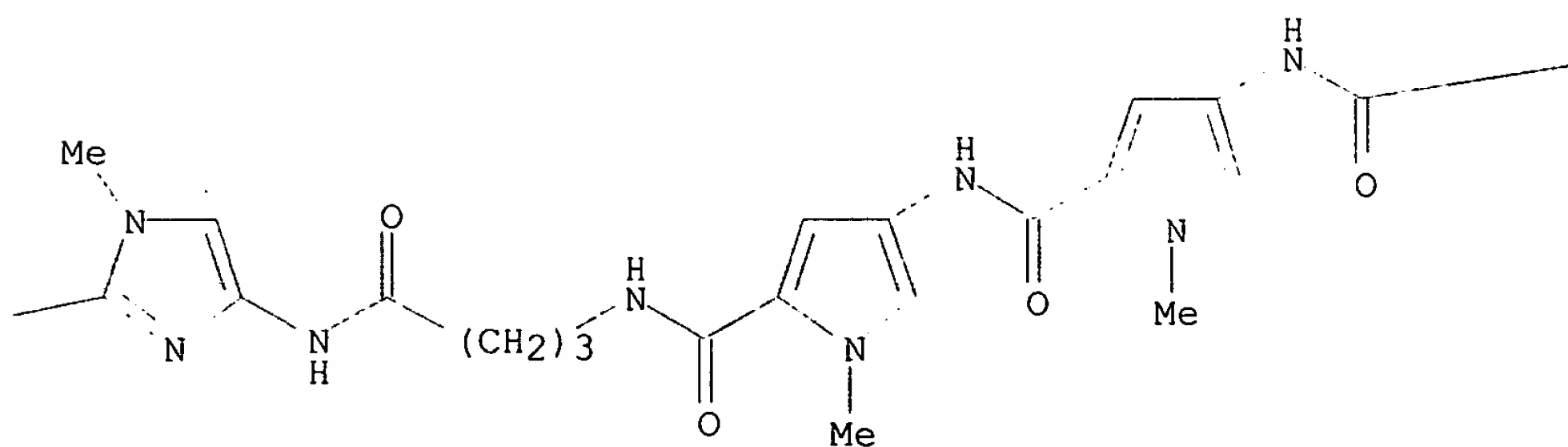
Absolute stereochemistry.

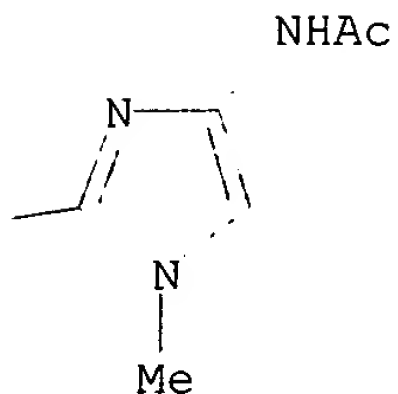
Double bond geometry as shown.

PAGE 1-A



PAGE 1-B





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

X REFERENCE 1: 139:276894

REFERENCE 2: 138:132742

L11 ANSWER 8 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 491647-63-3 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-oxobutyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)

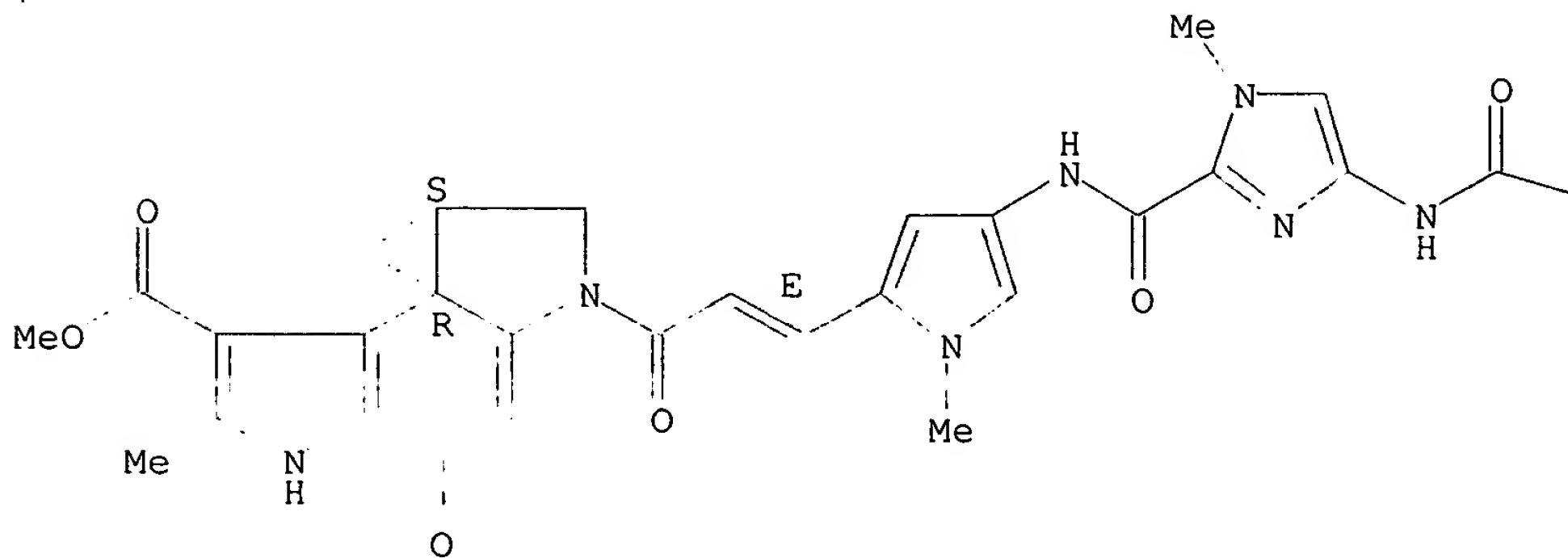
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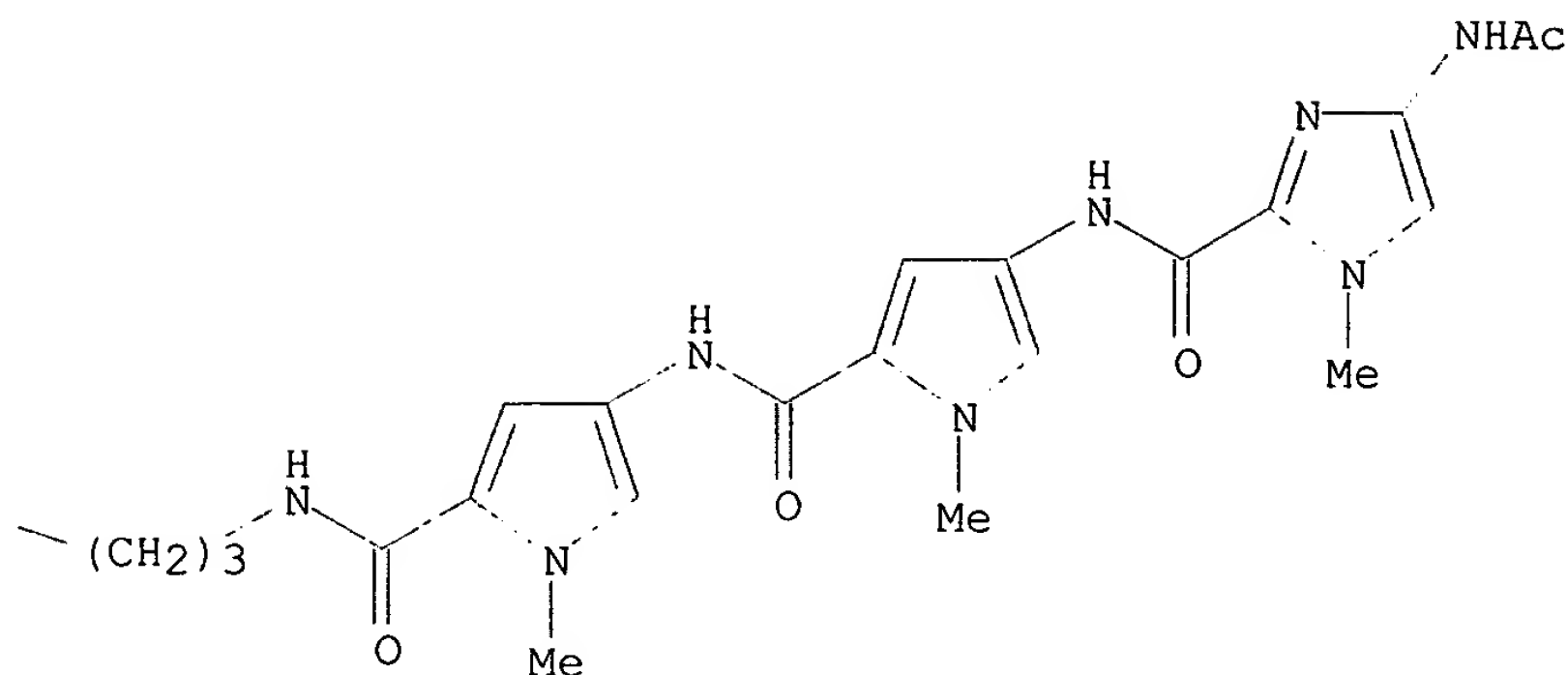
MF C50 H53 N15 O10

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:276894

REFERENCE 2: 139:30289

REFERENCE 3: 138:132742

L11 ANSWER 9 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 484017-86-9 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI)
(CA INDEX NAME)

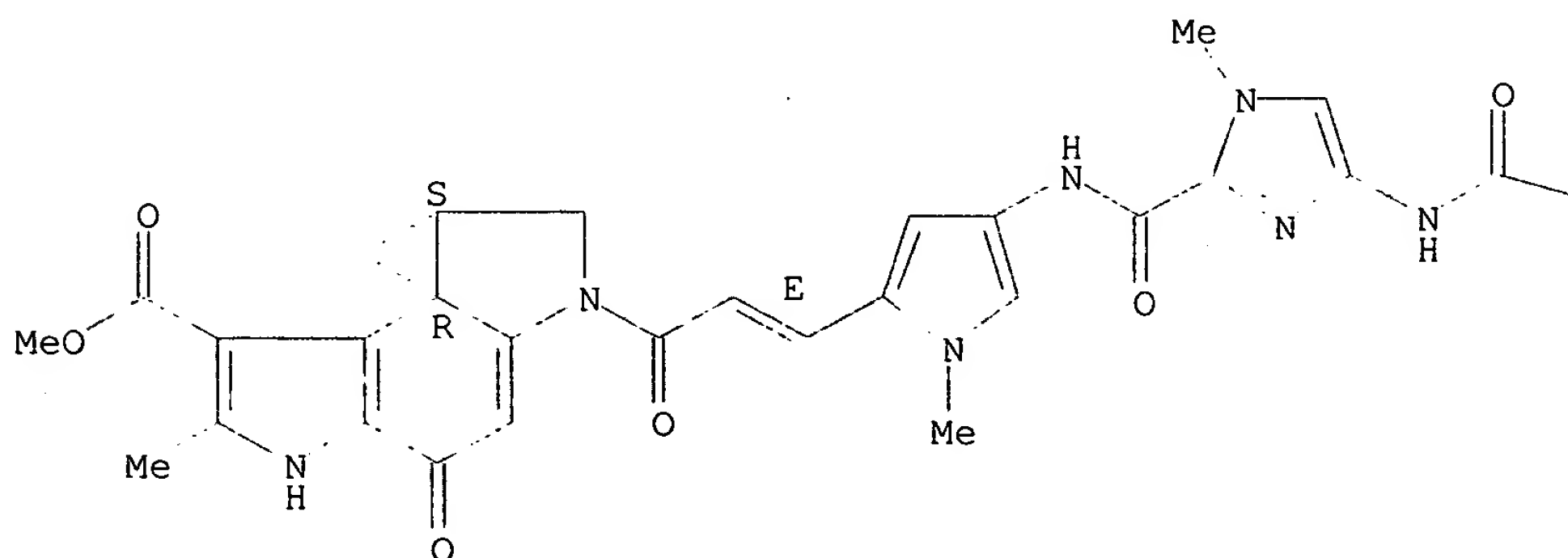
FS STEREOSEARCH

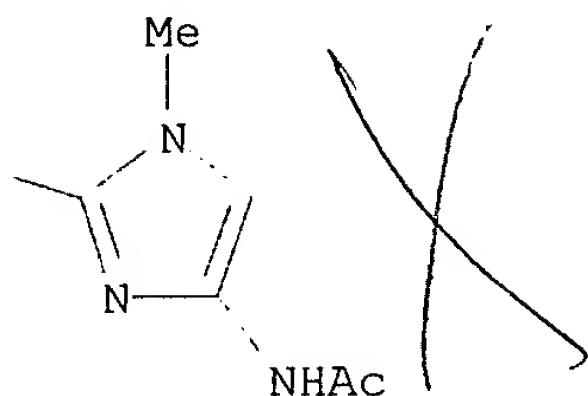
MF C34 H34 N10 O7

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





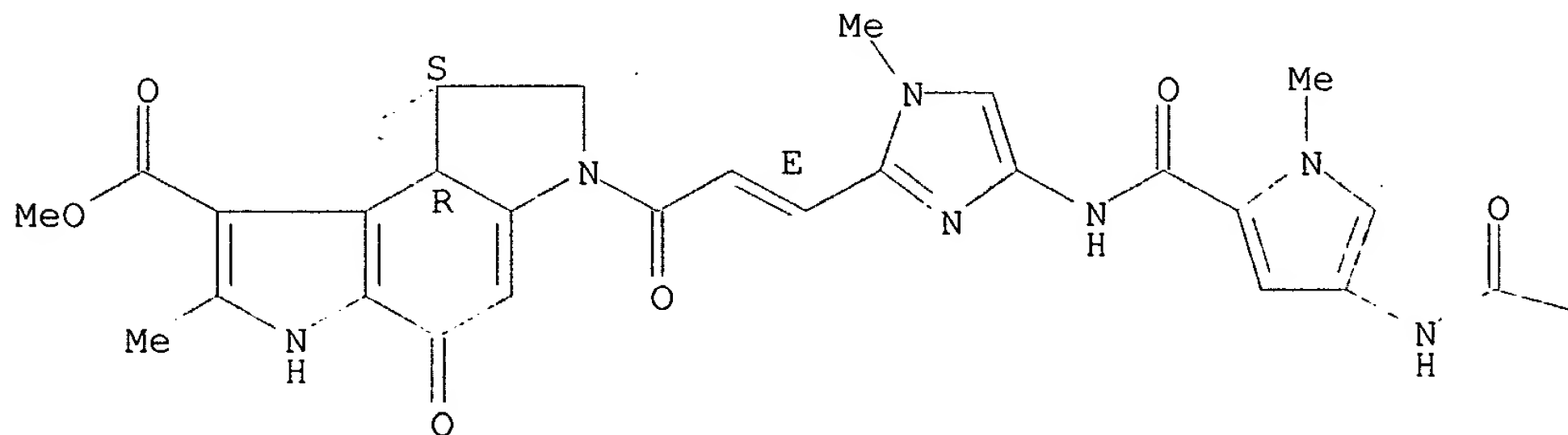
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

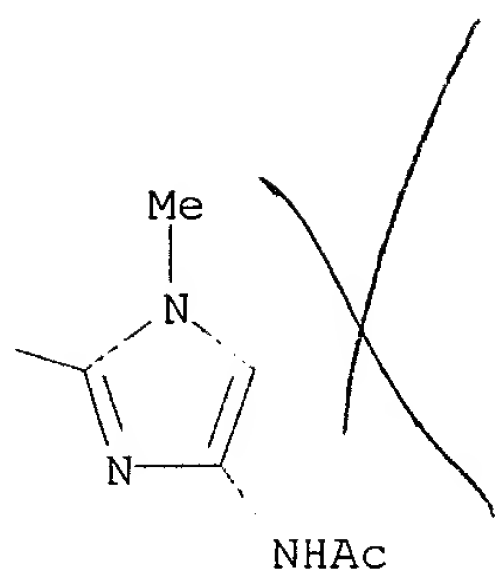
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:85083

L11 ANSWER 10 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 484017-85-8 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-
[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-
pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-imidazol-2-yl]-1-oxo-2-propenyl]-
1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C34 H34 N10 O7
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry as shown.





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:85083.

L11 ANSWER 11 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 373362-27-7 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-
[carbonylbis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-
1H-pyrrole-4,2-diyl)][(2E)-1-oxo-2-propene-3,1-diyl]]bis[1,2,4,5,8,8a-
hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA
INDEX NAME)

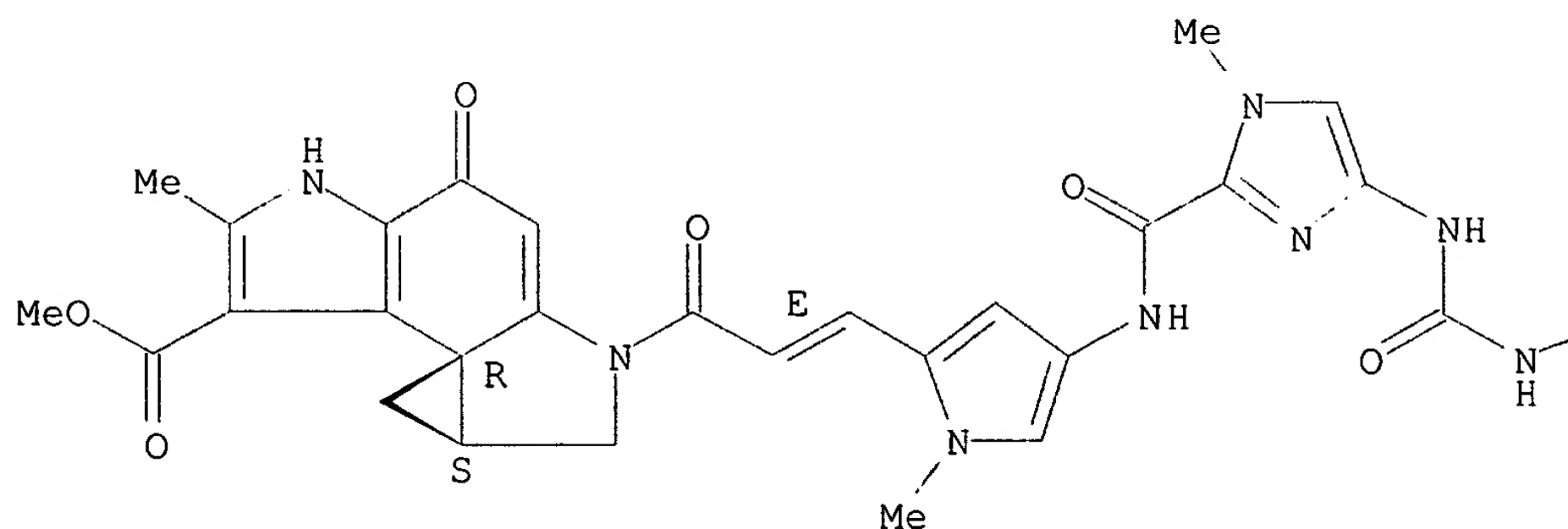
FS STEREOSEARCH

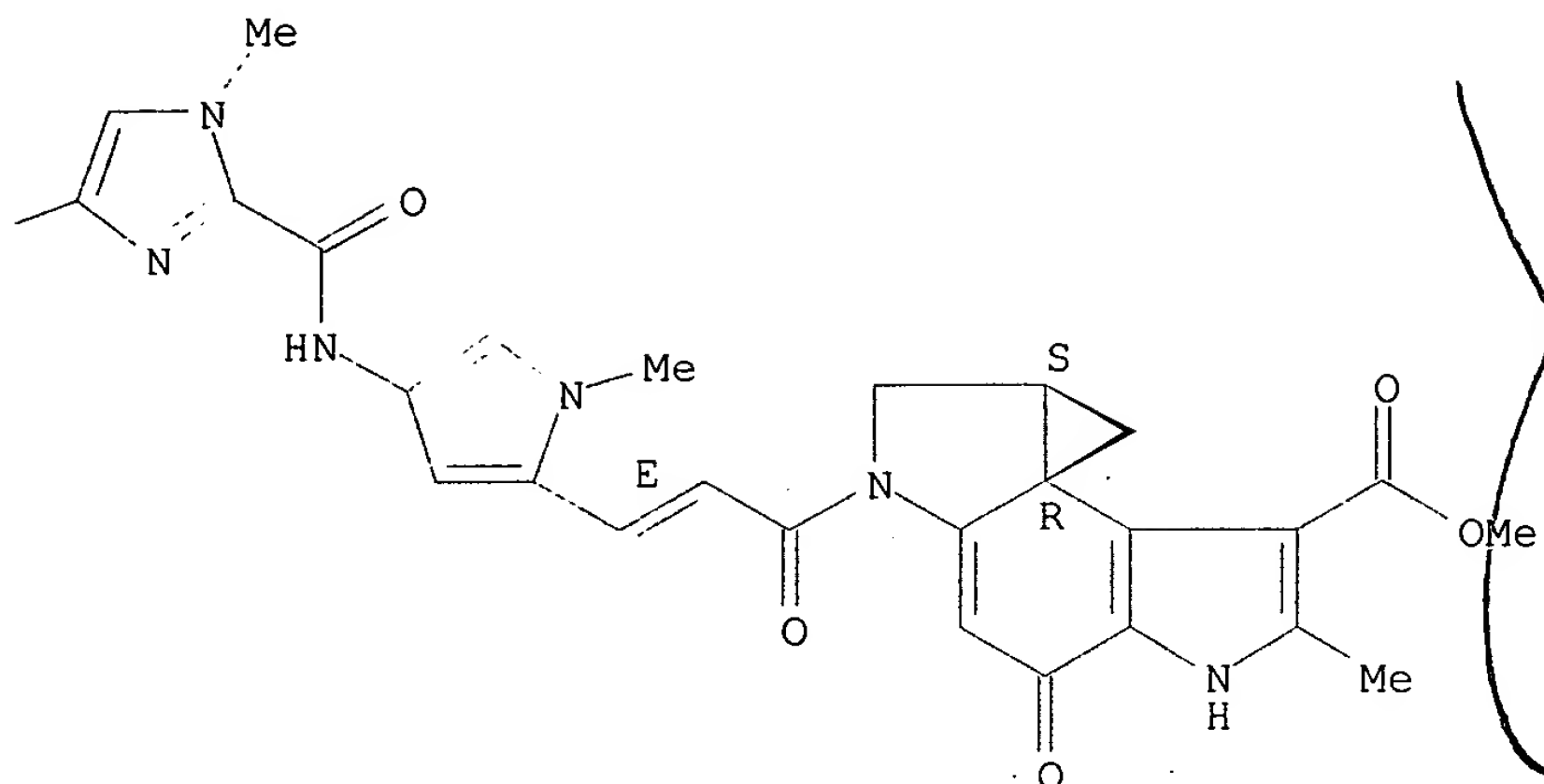
MF C55 H52 N14 O11

SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

L11 ANSWER 12 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 373362-26-6 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,4-dioxo-2-butene-1,4-diyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)][(2E)-1-oxo-2-propene-3,1-diyl]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C58 H54 N14 O12

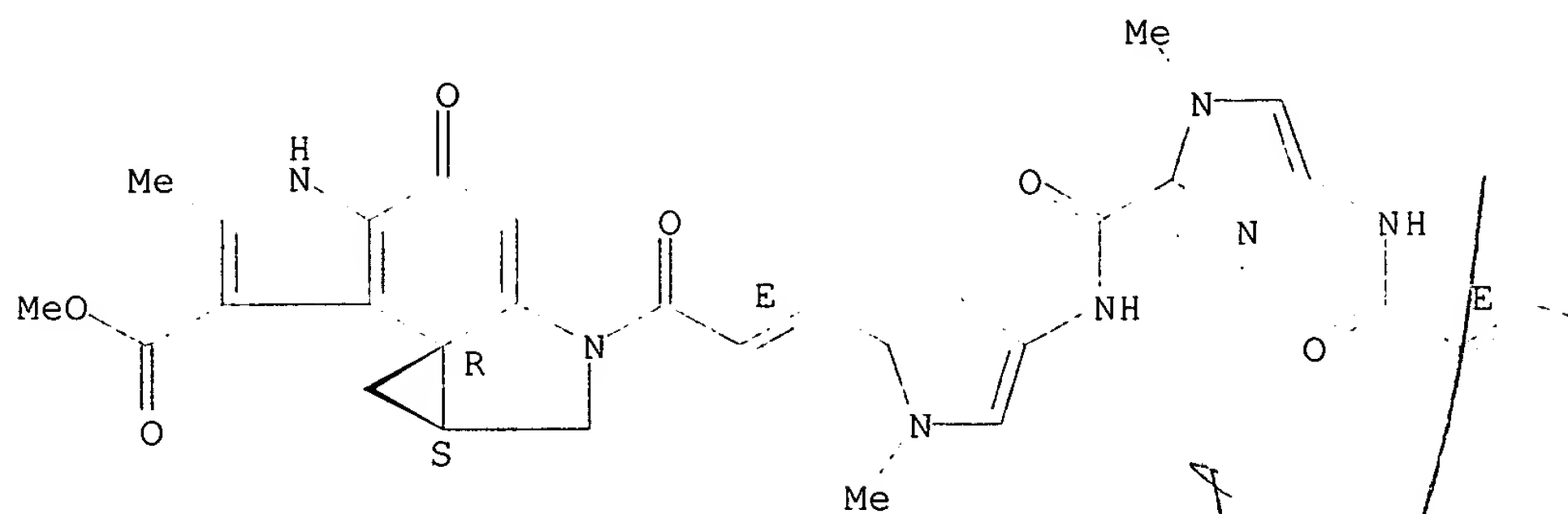
SR CA

LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

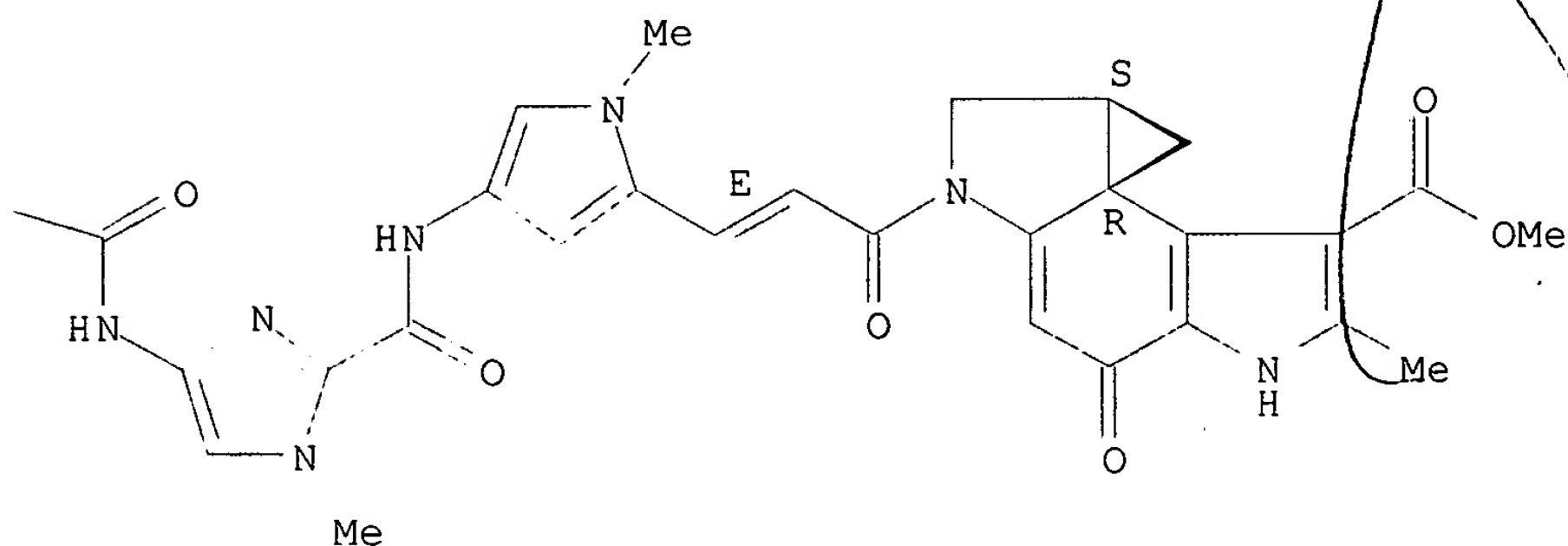
Absolute stereochemistry.

Double bond geometry as shown.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

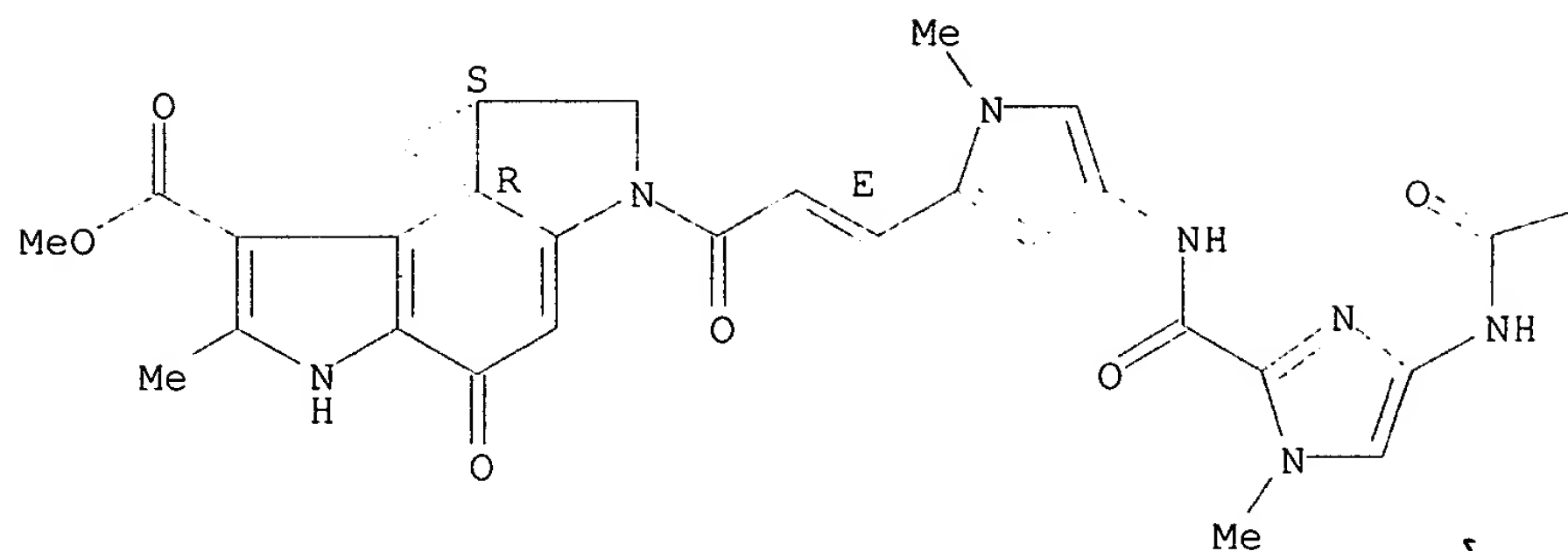
REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

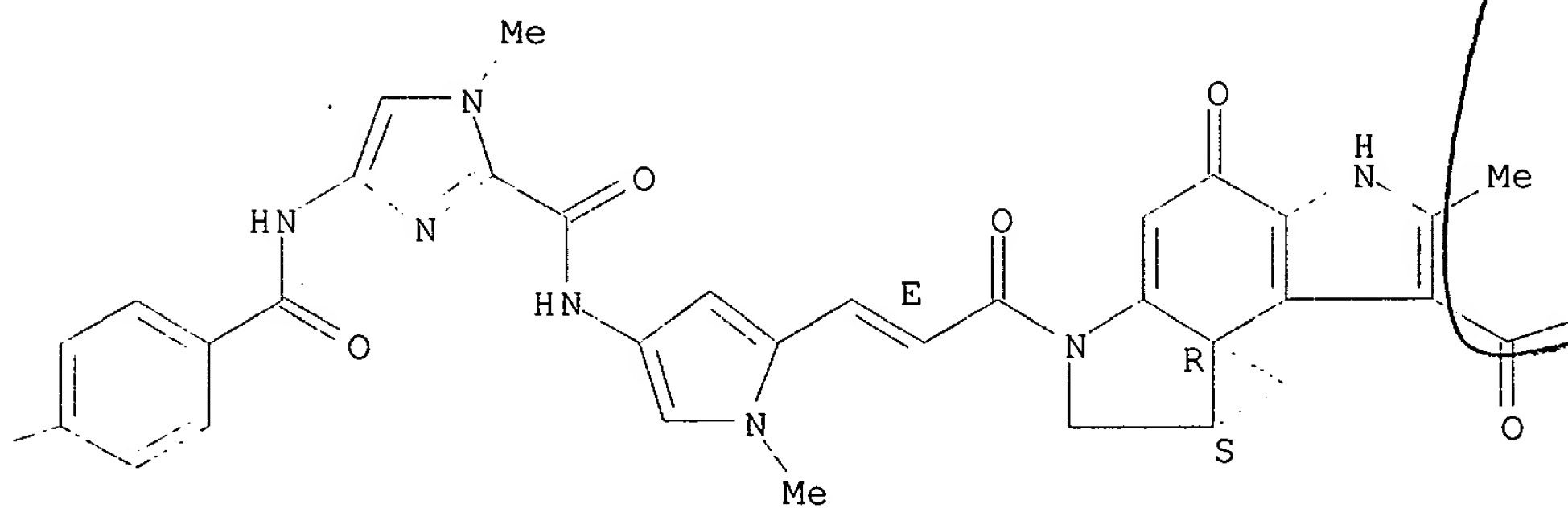
L11 ANSWER 13 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 373362-24-4 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,4-phenylenebis(carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl))[(2E)-1-oxo-2-propene-3,1-diyl]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C62 H56 N14 O12
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A



PAGE/ 1-B



PAGE 1-C

 OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

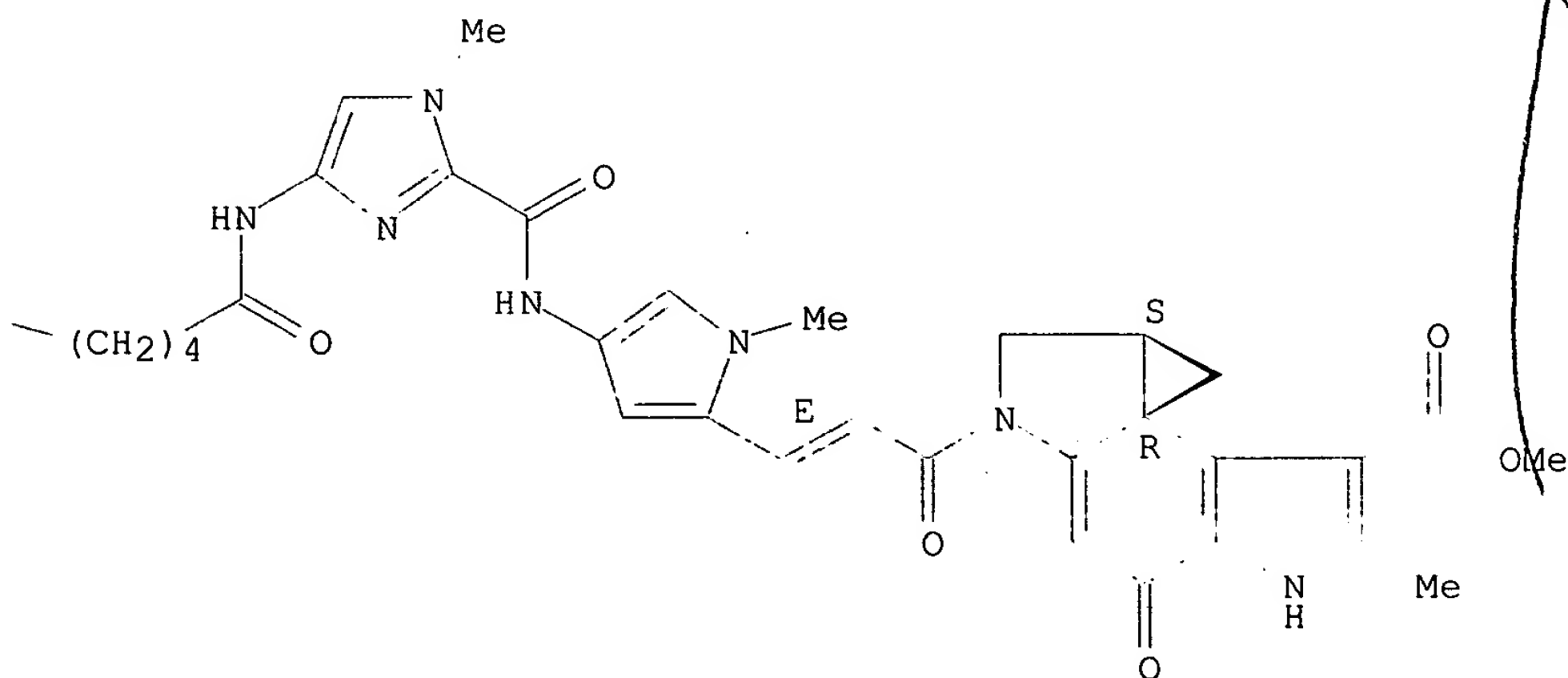
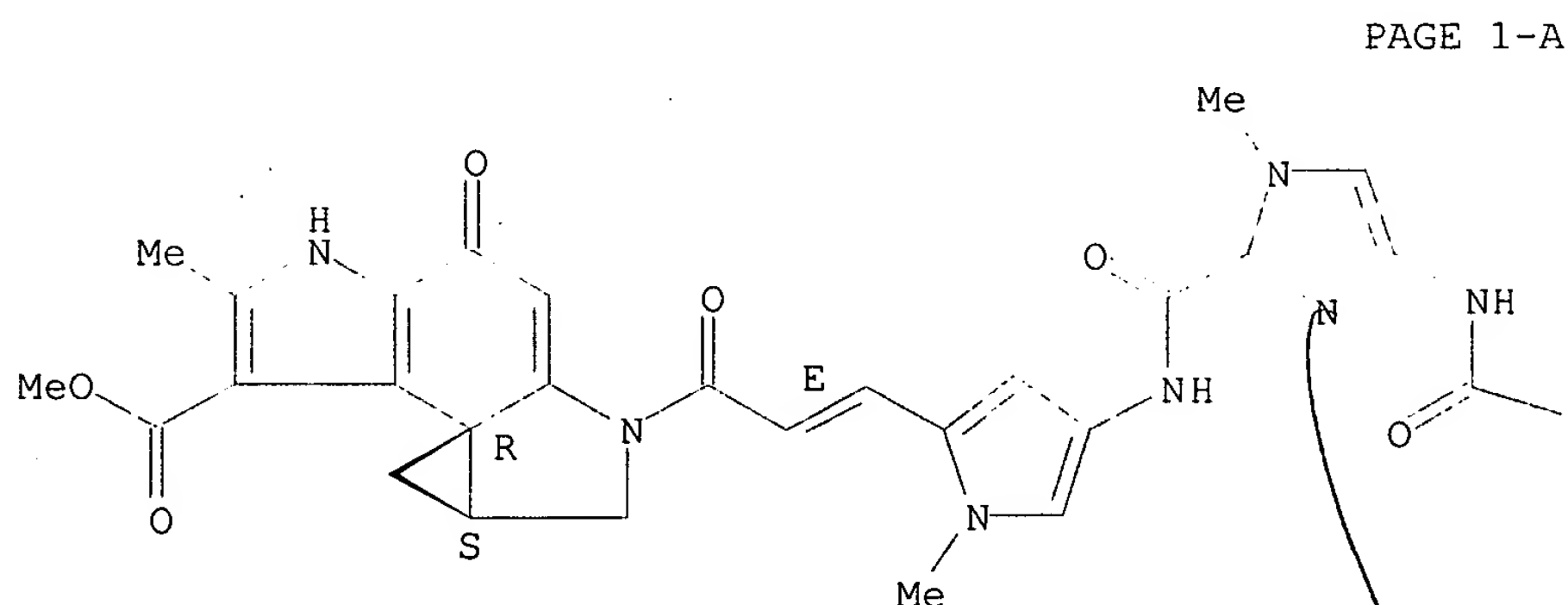
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

L11 ANSWER 14 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 373362-22-2 REGISTRY
 CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,6-dioxo-1,6-hexanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)][(2E)-1-oxo-2-propene-3,1-diyl]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C60 H60 N14 O12
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Absolute stereochemistry.
 Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 138:333279

REFERENCE 2: 135:371743

L11 ANSWER 15 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 349647-83-2 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,4-phenylenebis(carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl))]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

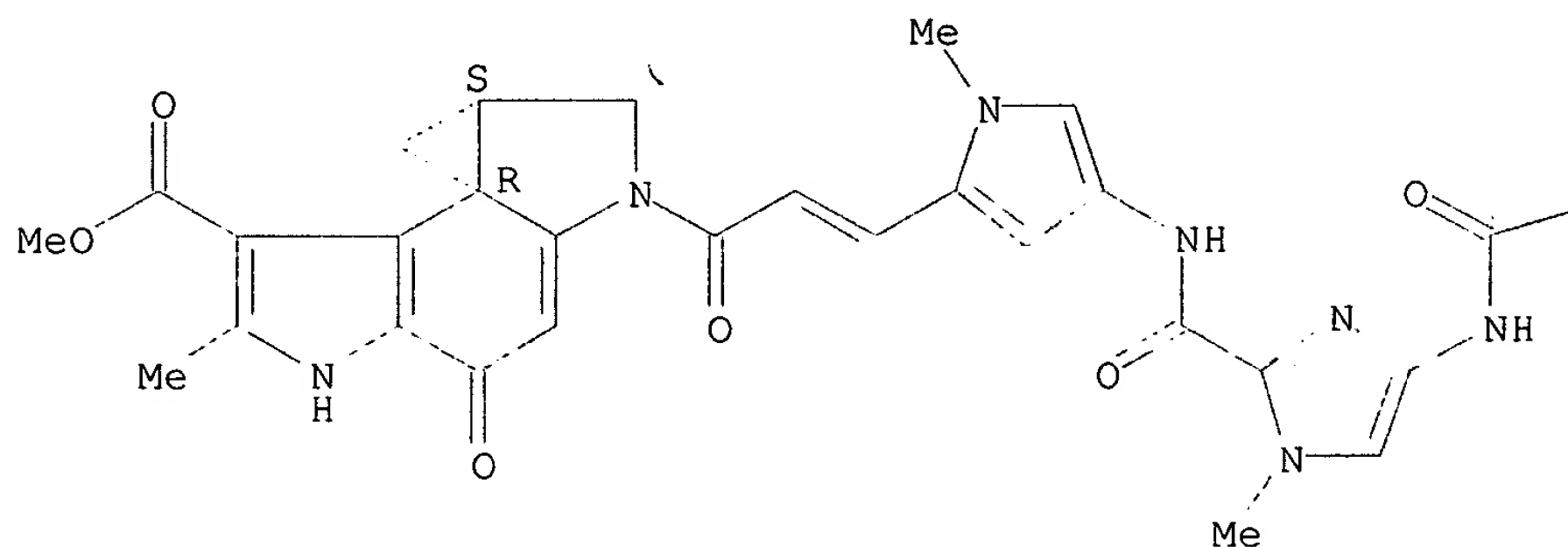
MF C62 H56 N14 O12

SR CA

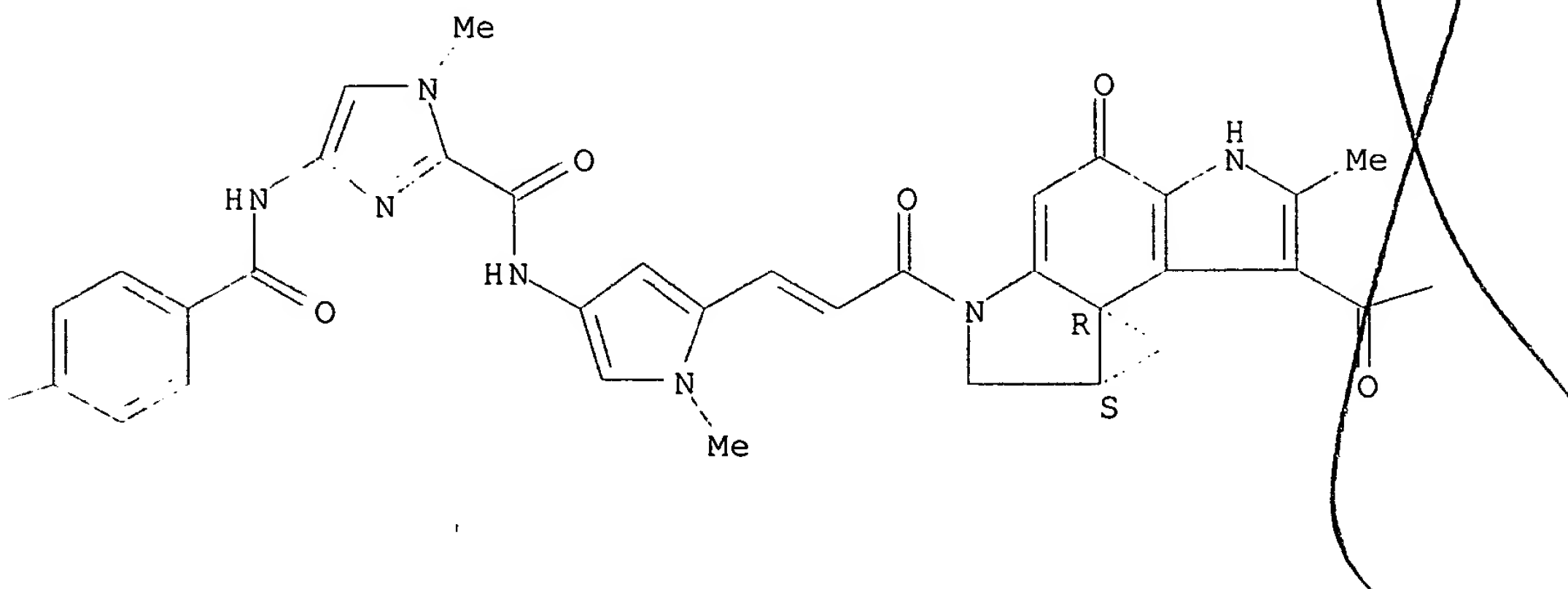
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

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—OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

L11 ANSWER 16 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 349647-82-1 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[1,3-phenylenebis(carbonylimino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl))]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C62 H56 N14 O12

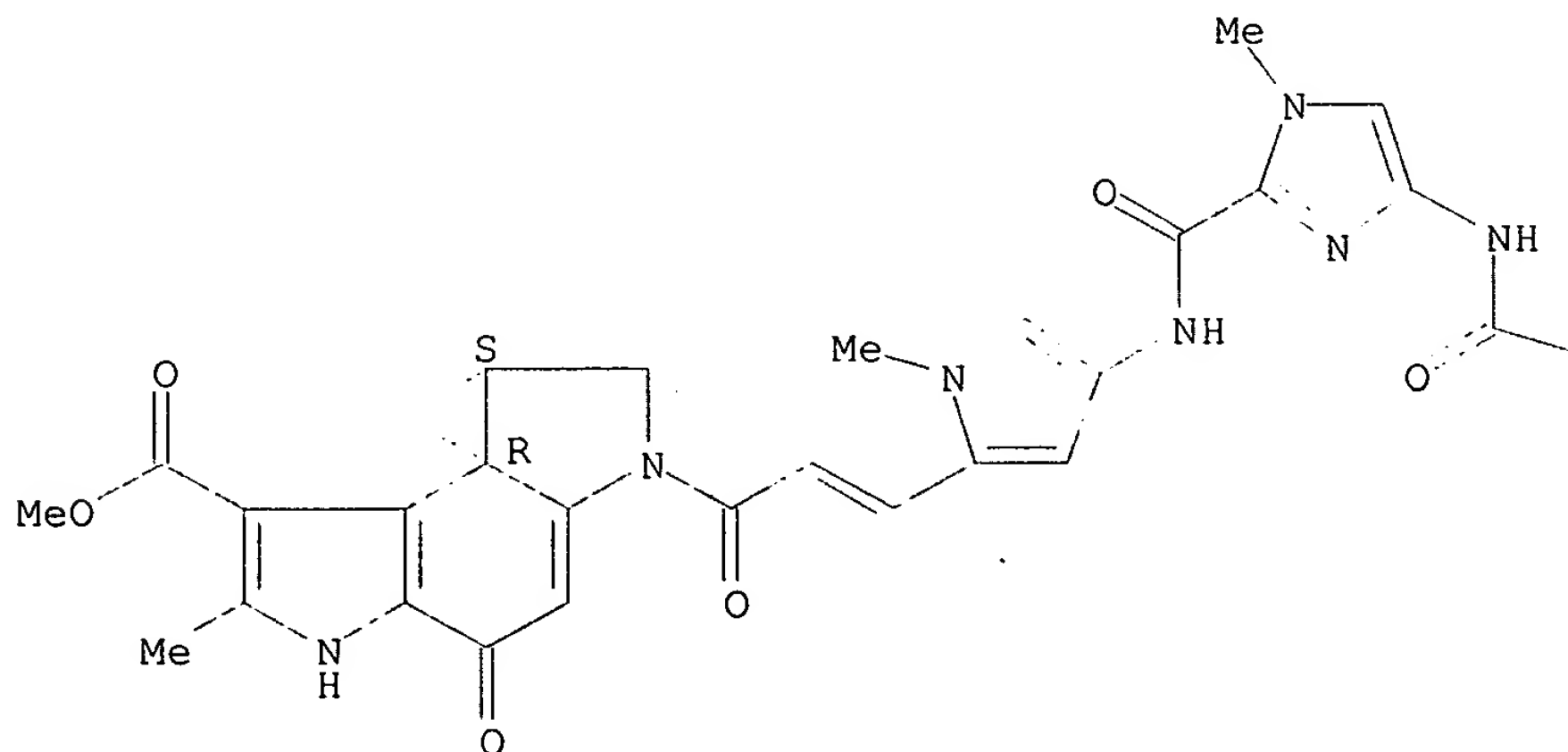
SR CA

LC STN Files: CA, CAPLUS

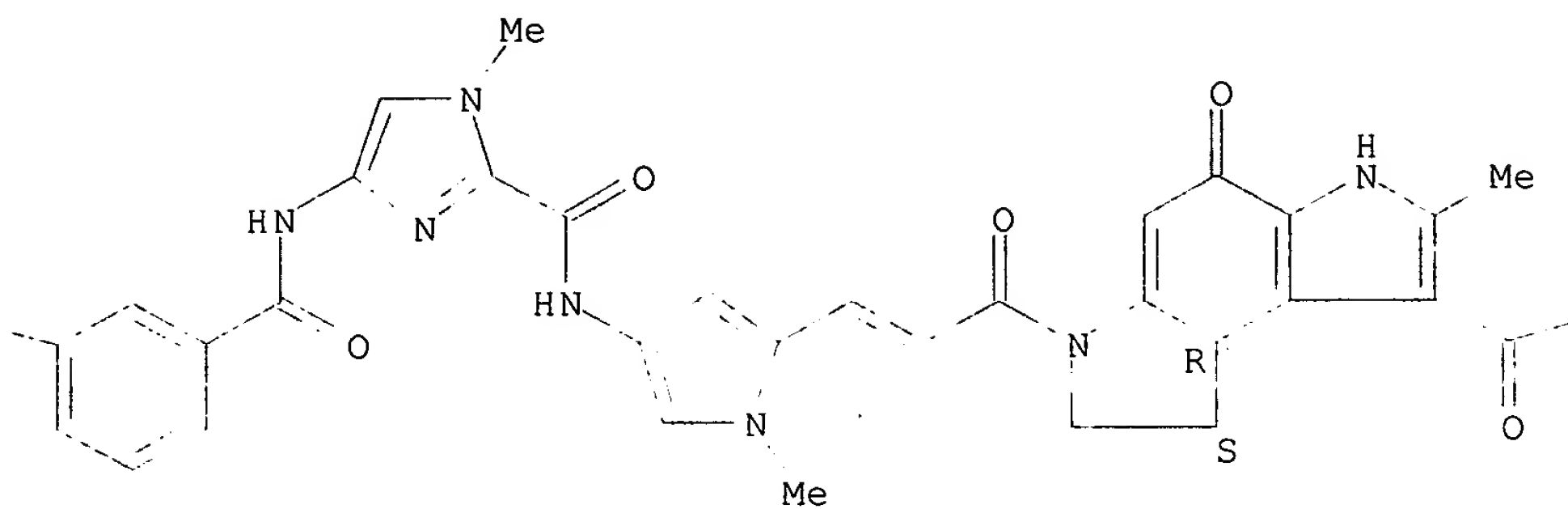
Absolute stereochemistry.

Double bond geometry unknown.

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OMe

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

L11 ANSWER 17 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 349647-81-0 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,6-dioxo-1,6-hexanediyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C60 H60 N14 O12

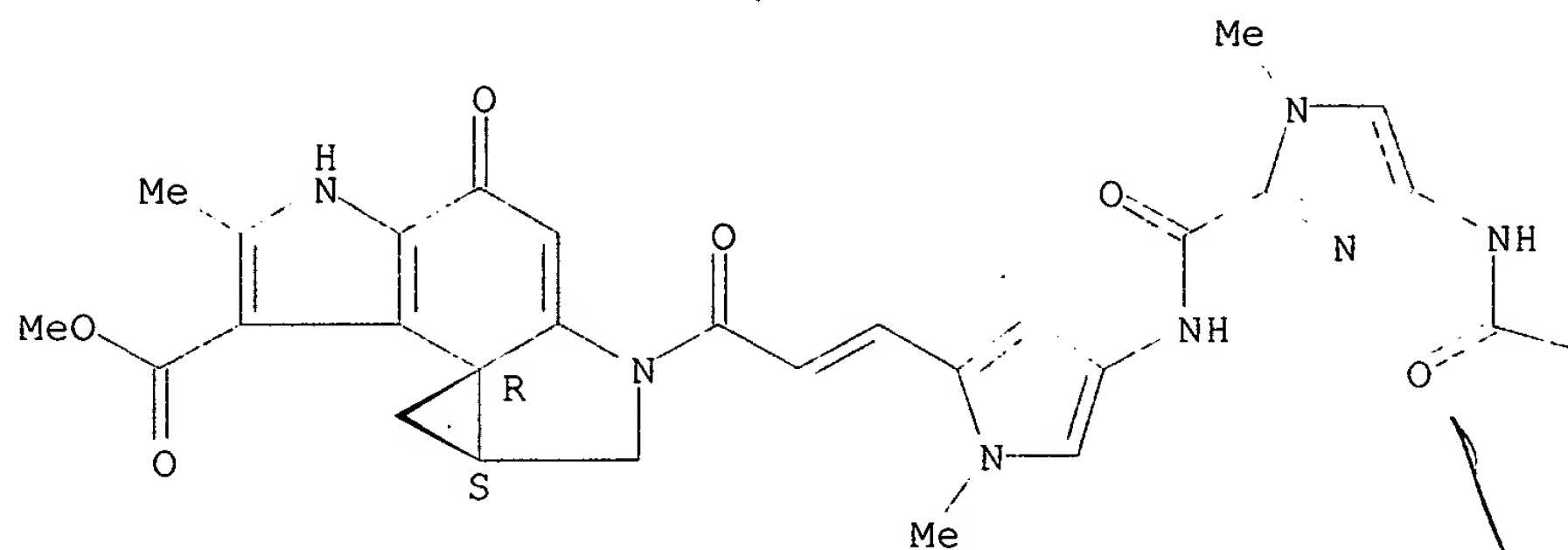
SR CA

LC STN Files: CA, CAPLUS

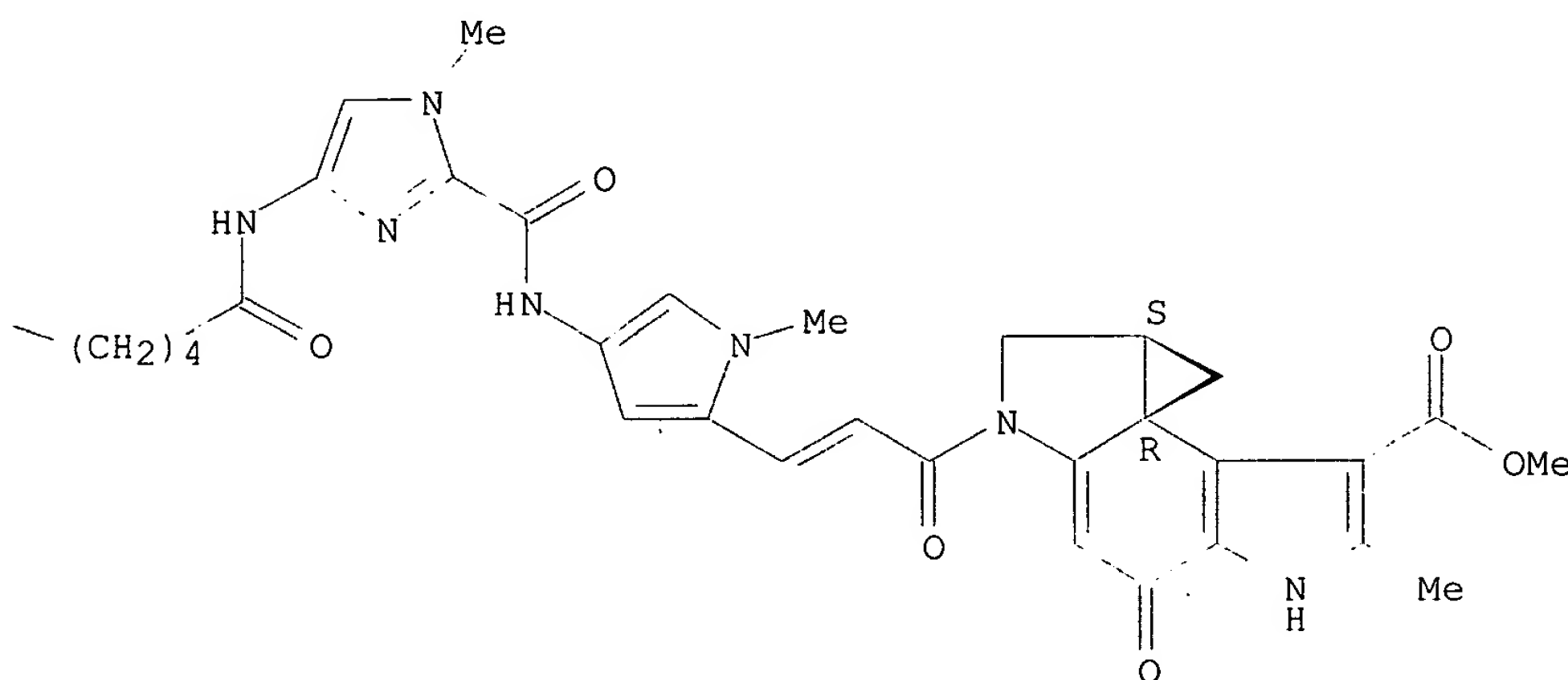
Absolute stereochemistry.

Double bond geometry unknown.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

L11 ANSWER 18 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 349647-80-9 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,5-dioxo-1,5-pentanediy)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C59 H58 N14 O12

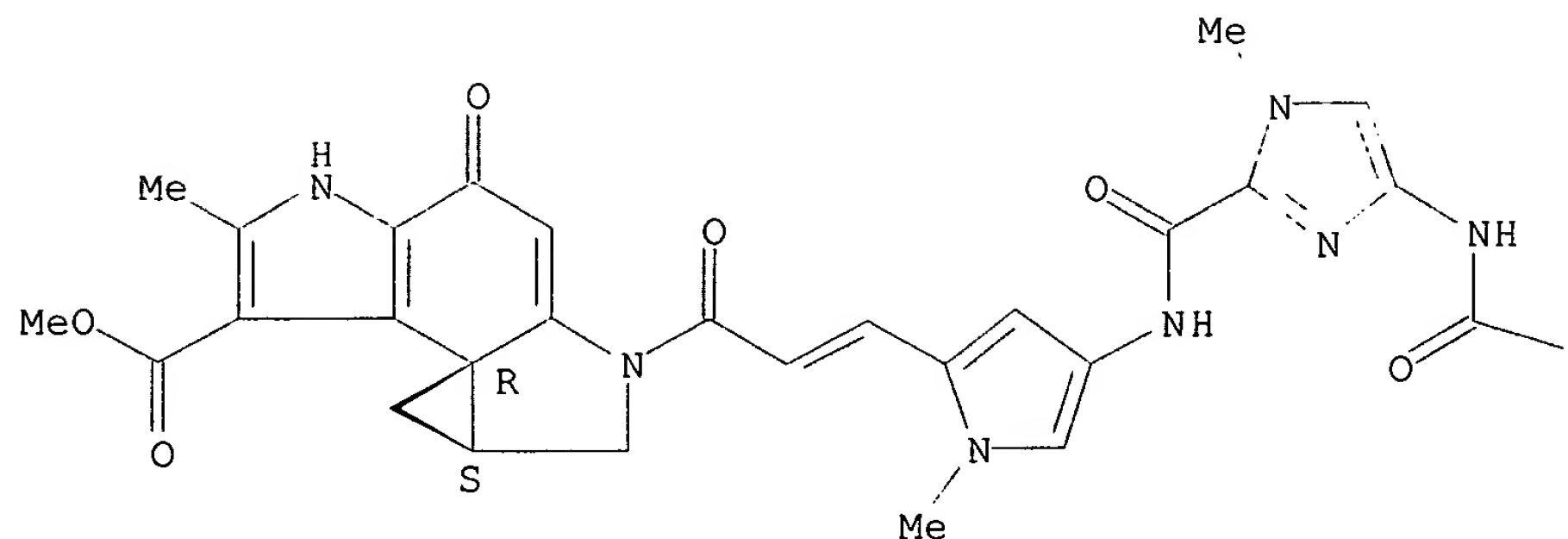
SR CA

LC STN Files: CA, CAPLUS

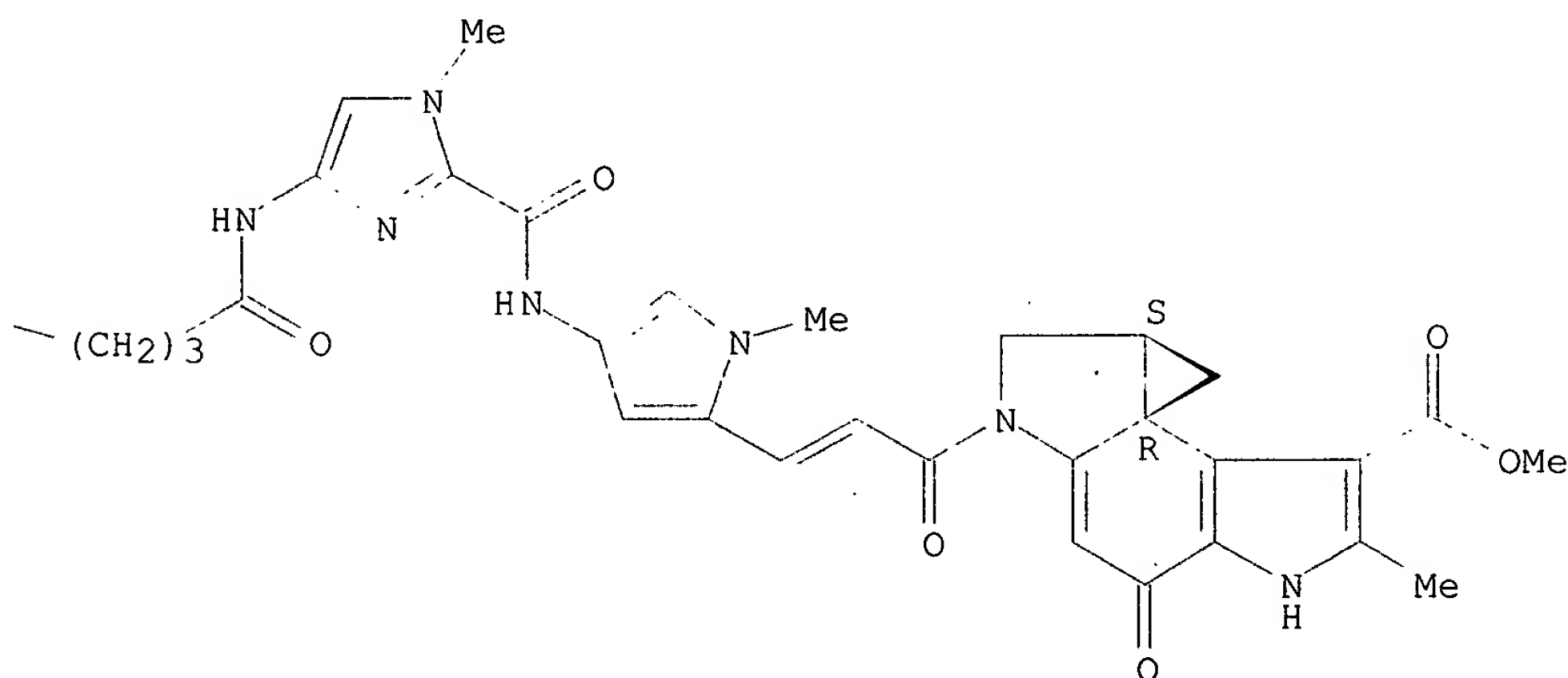
Absolute stereochemistry.

Double bond geometry unknown.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

L11 ANSWER 19 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 349647-79-6 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-[(1,4-dioxo-2-butene-1,4-diyl)bis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C58 H54 N14 O12

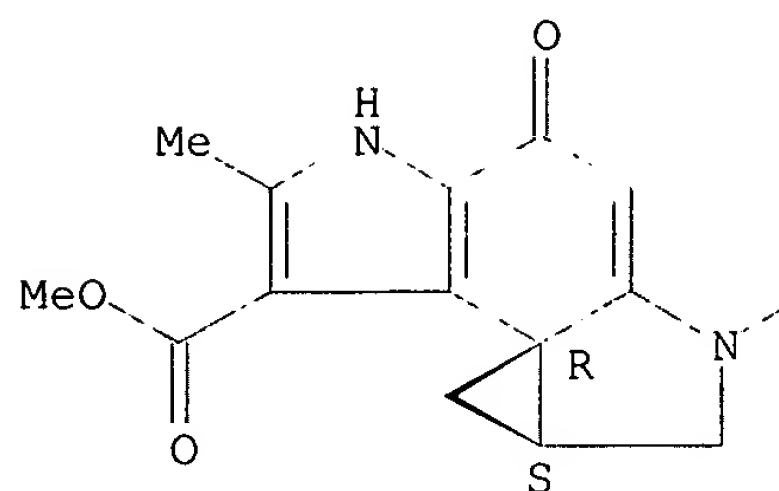
SR CA

LC STN Files: CA, CAPLUS

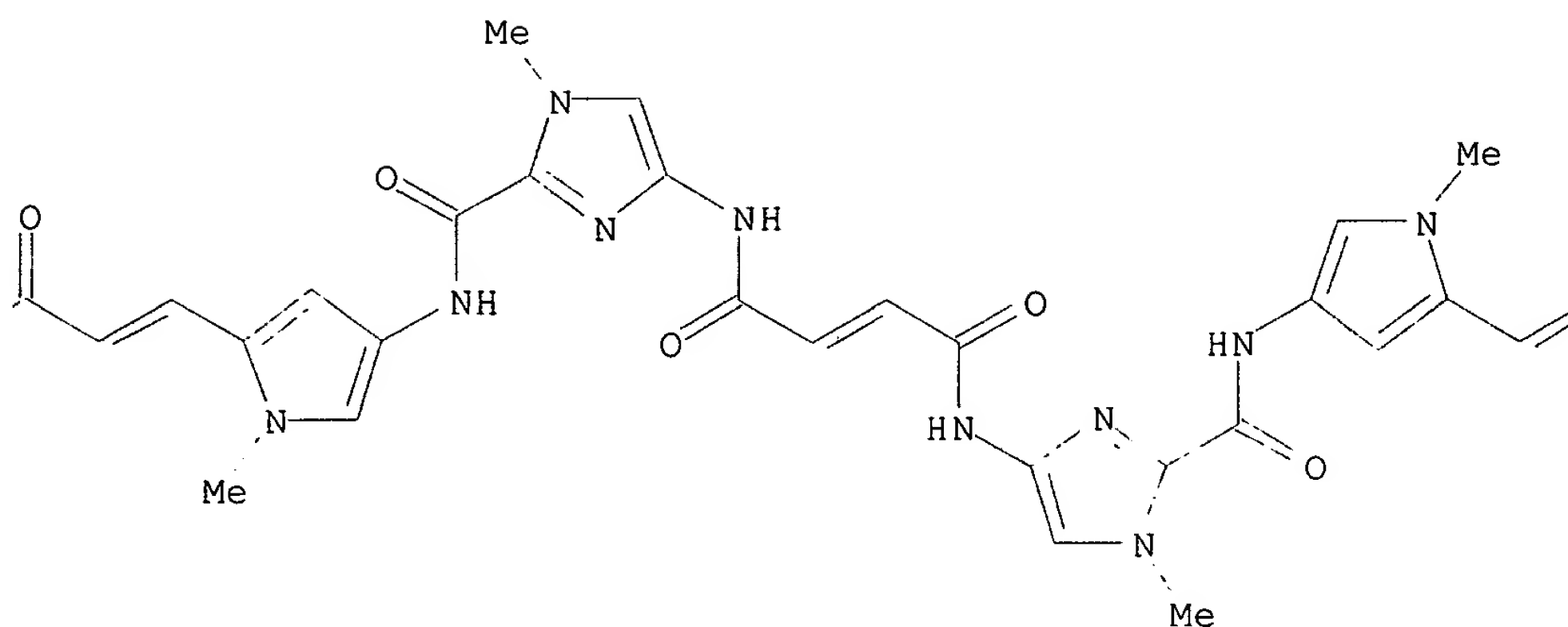
Absolute stereochemistry.

Double bond geometry unknown.

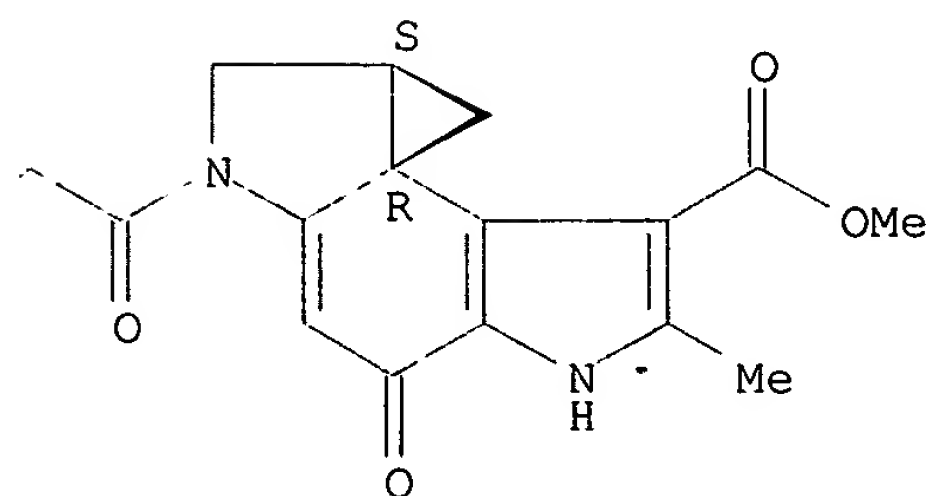
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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

L11 ANSWER 20 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 349647-78-5 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2,2'-
[carbonylbis[imino(1-methyl-1H-imidazole-4,2-diyl)carbonylimino(1-methyl-
1H-pyrrole-4,2-diyl)(1-oxo-2-propene-3,1-diyl)]]bis[1,2,4,5,8,8a-hexahydro-
6-methyl-4-oxo-, dimethyl ester, (7bR,7'bR,8aS,8'aS)- (9CI) (CA INDEX
NAME)

FS STEREOSEARCH

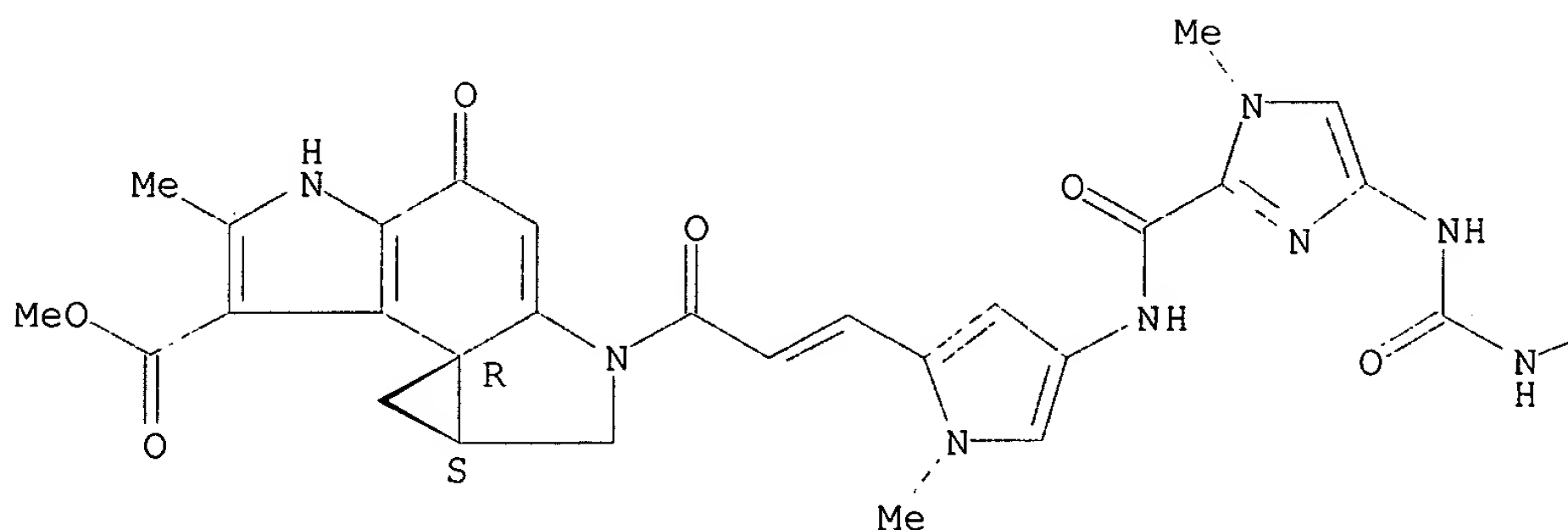
MF C55 H52 N14 O11

SR CA

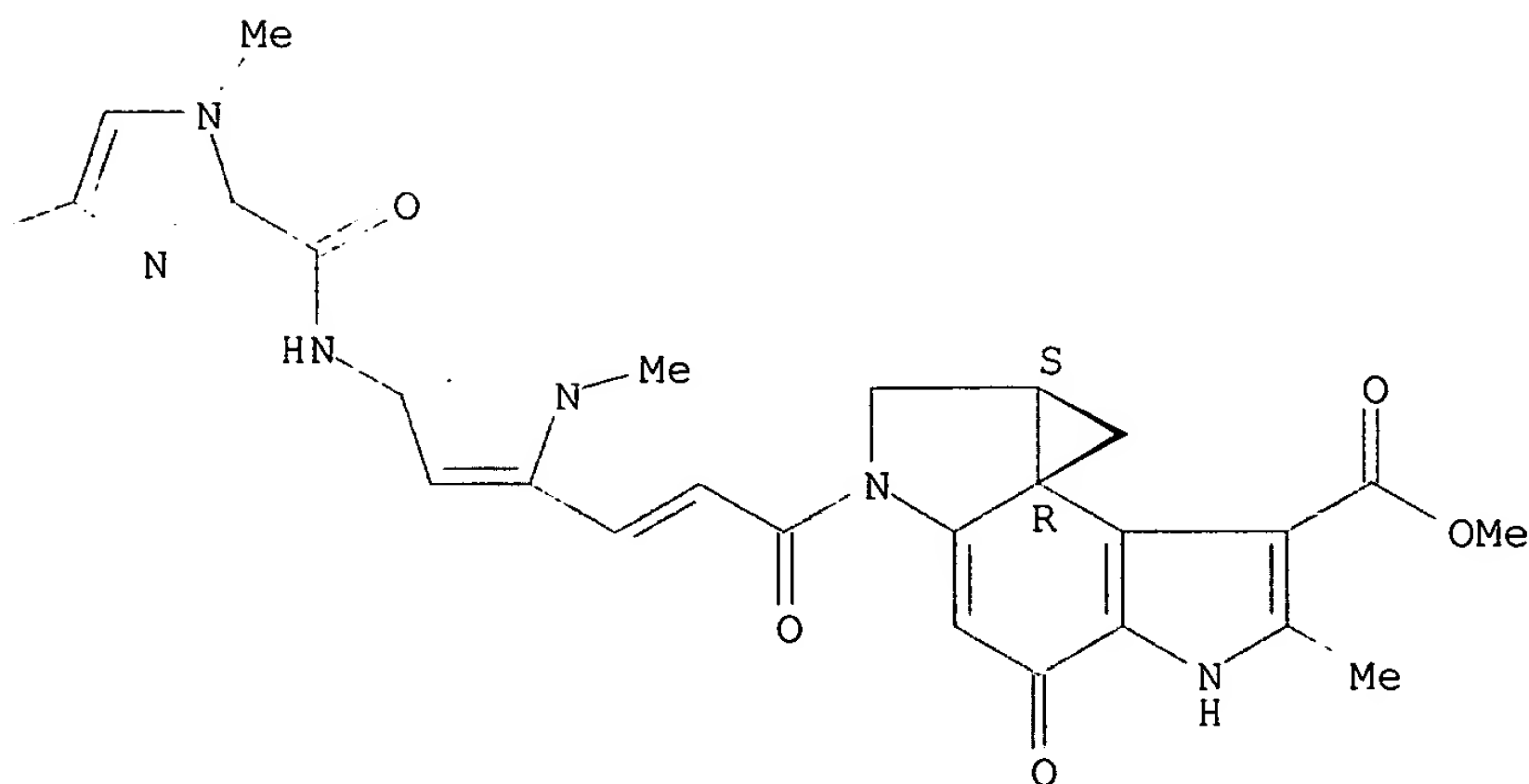
LC STN Files: CA, CAPLUS

Absolute stereochemistry.
Double bond geometry unknown.

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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

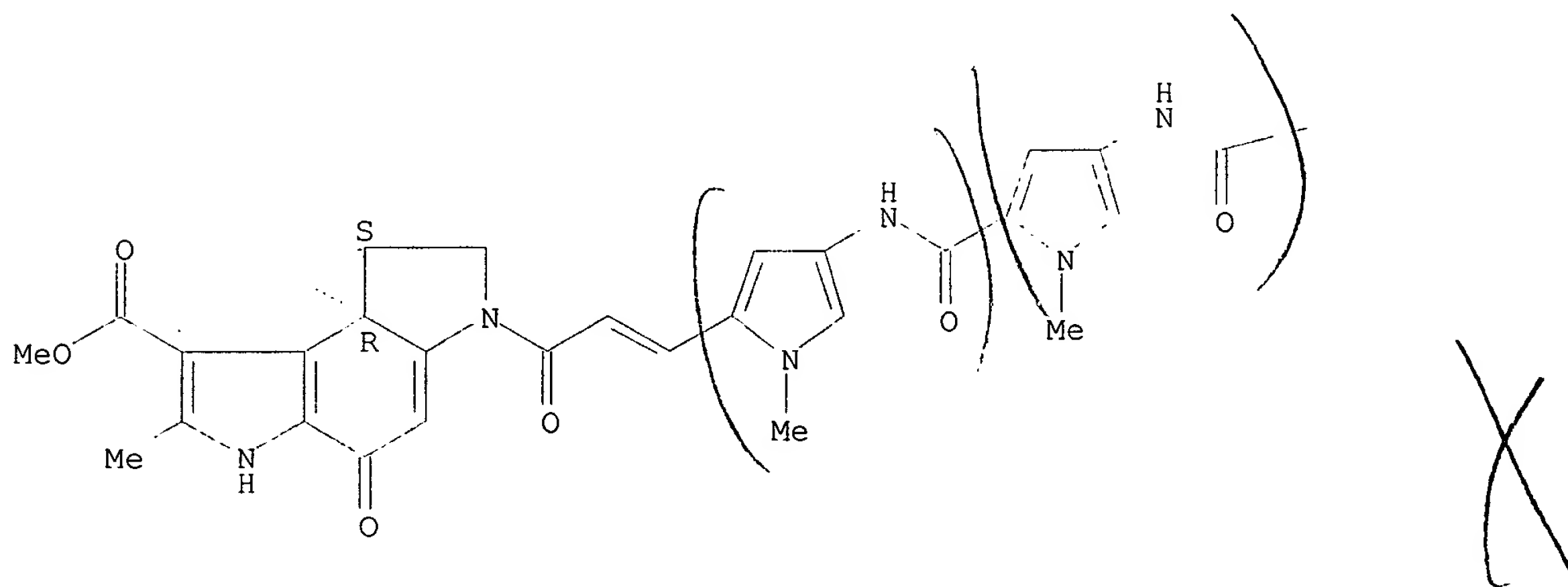
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 135:102536

L11 ANSWER 21 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 339984-92-8 REGISTRY
 CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-[[[4-(acetylamino)-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C36 H36 N8 O7
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

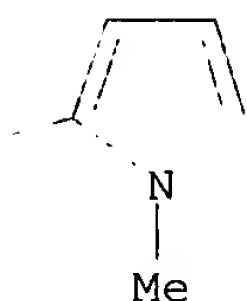
Absolute stereochemistry.
 Double bond geometry unknown.

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NHAc



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

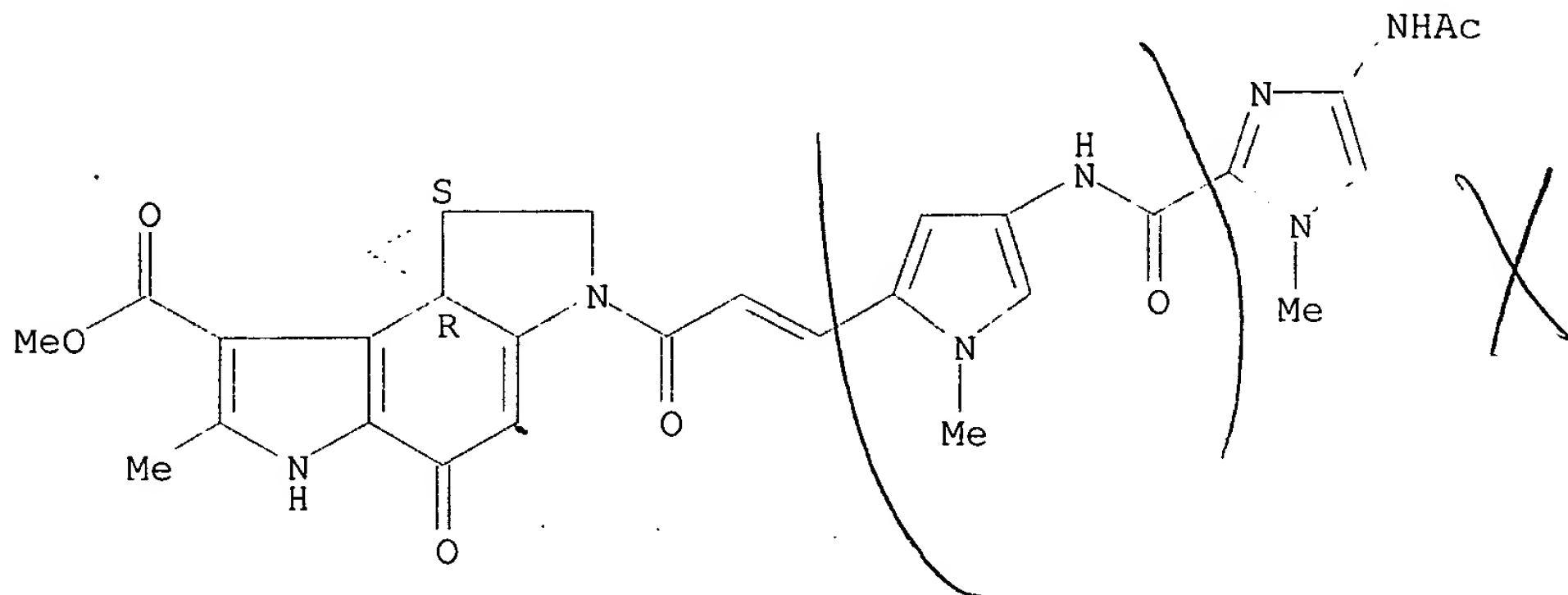
REFERENCE 1: 134:366795

L11 ANSWER 22 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 339984-91-7 REGISTRY
 CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-

(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH
MF C29 H29 N7 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

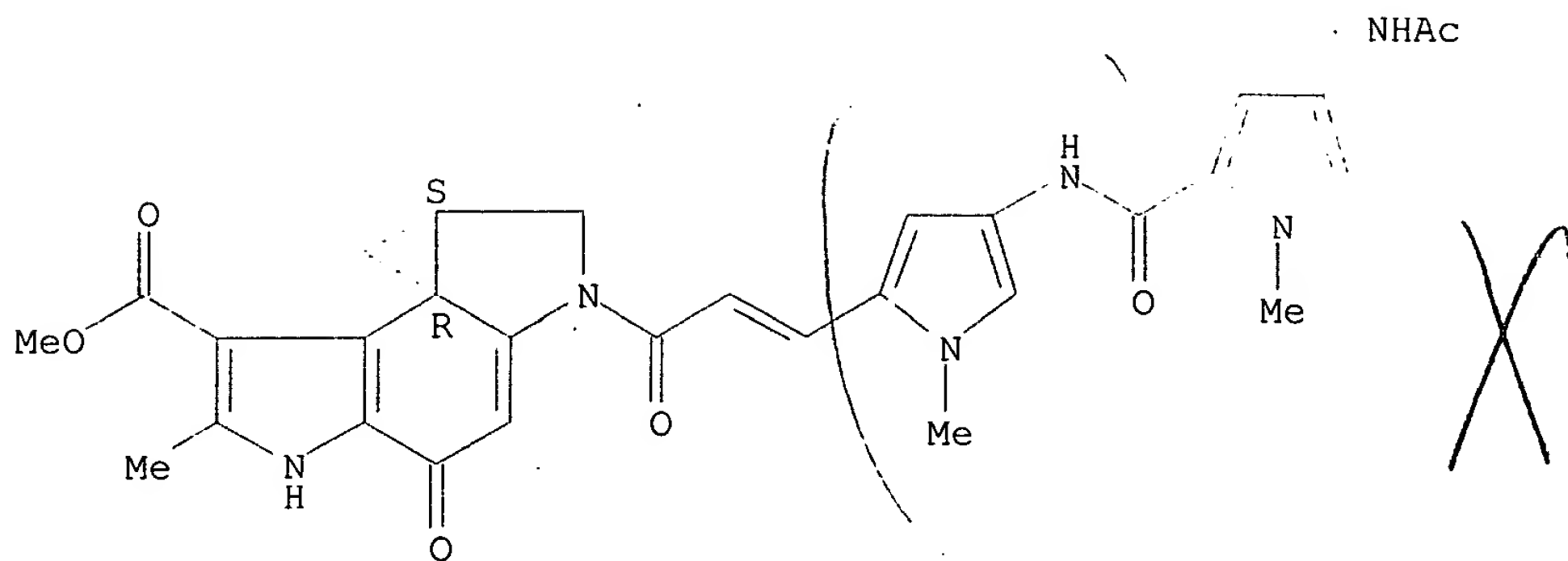
2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:345455

REFERENCE 2: 134:366795

L11 ANSWER 23 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 339984-88-2 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-(acetylamino)-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C30 H30 N6 O6
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:345455

REFERENCE 2: 134:366795

L11 ANSWER 24 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 296794-38-2 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-(acetylamino)-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)

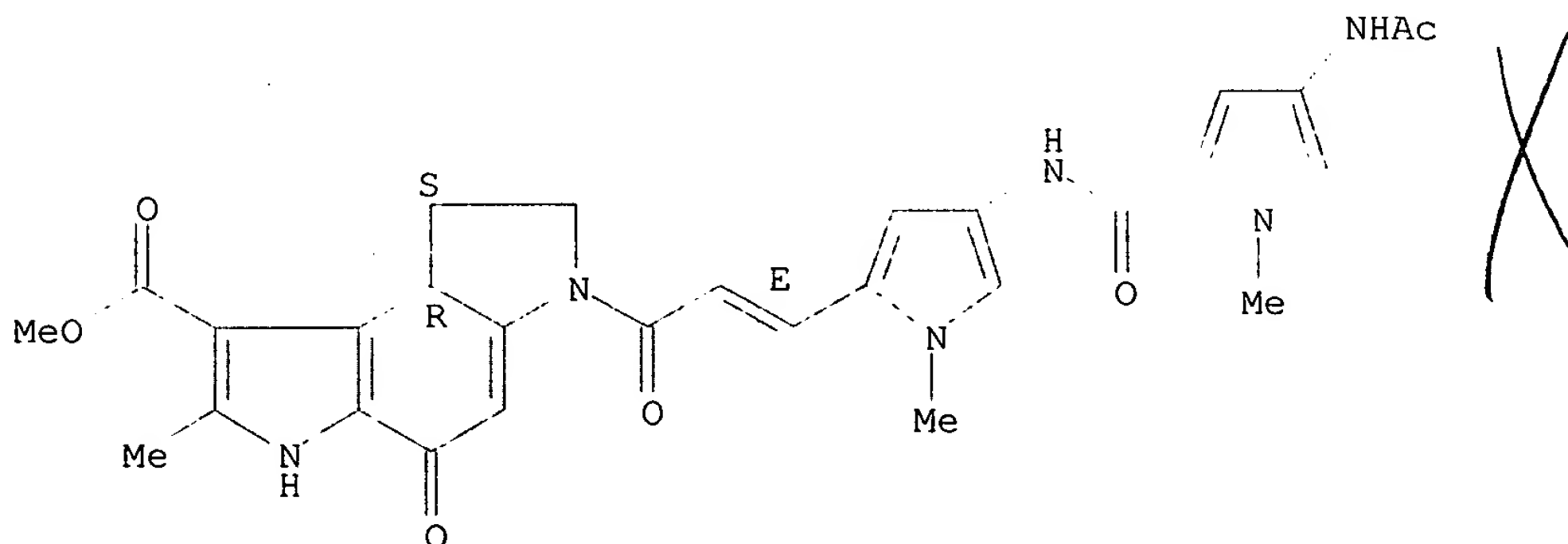
FS STEREOSEARCH

MF C30 H30 N6 O6

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.



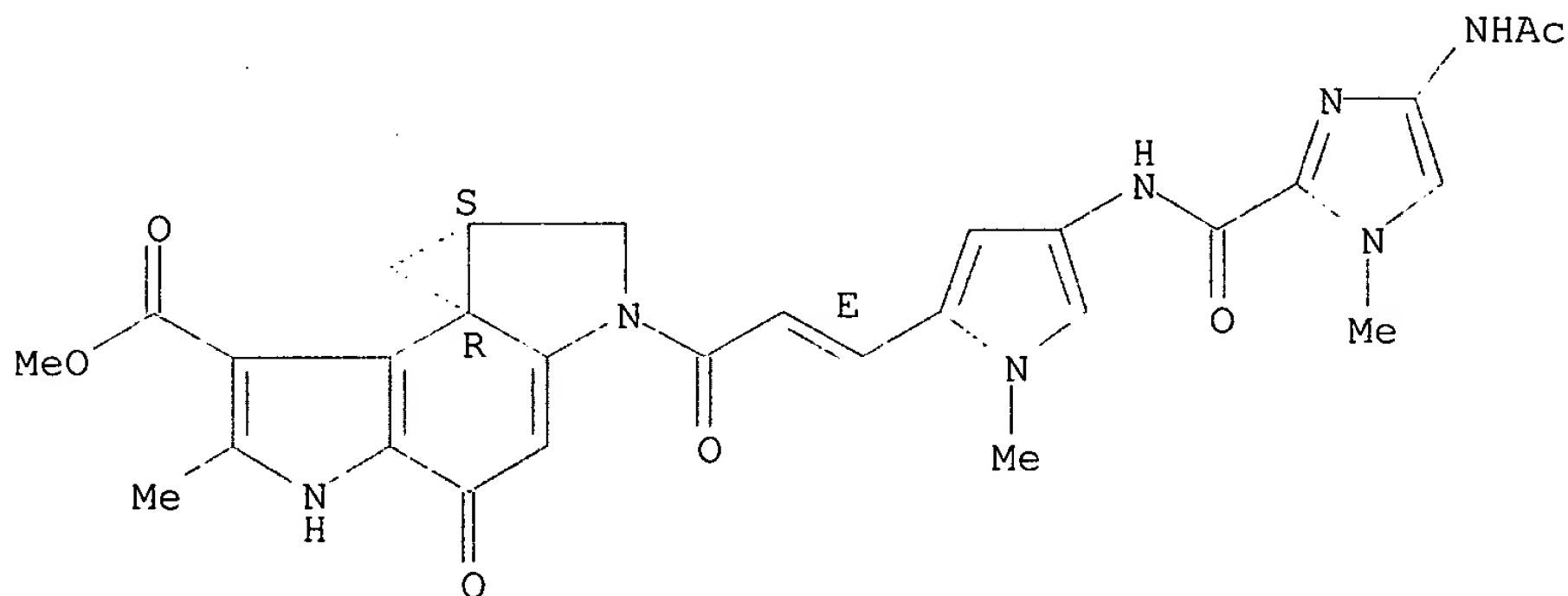
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:266852

L11 ANSWER 25 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 296794-37-1 REGISTRY
 CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)-(9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C29 H29 N7 O6
 SR CA
 LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
 Double bond geometry as shown.



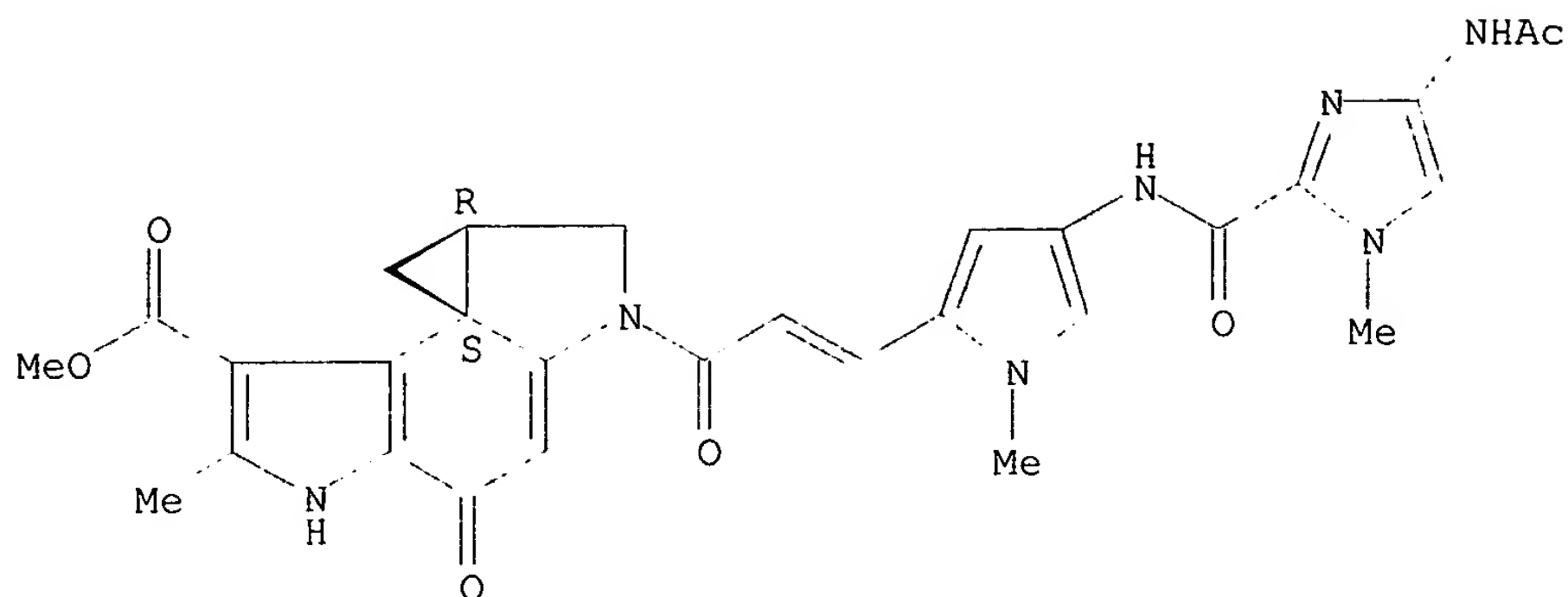
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 133:266852

L11 ANSWER 26 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 263710-69-6 REGISTRY
 CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-(acetylamino)-1-methyl-1H-imidazol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bS,8aR)-(9CI) (CA INDEX NAME)
 FS STEREOSEARCH
 MF C29 H29 N7 O6
 SR CA
 LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.
 Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

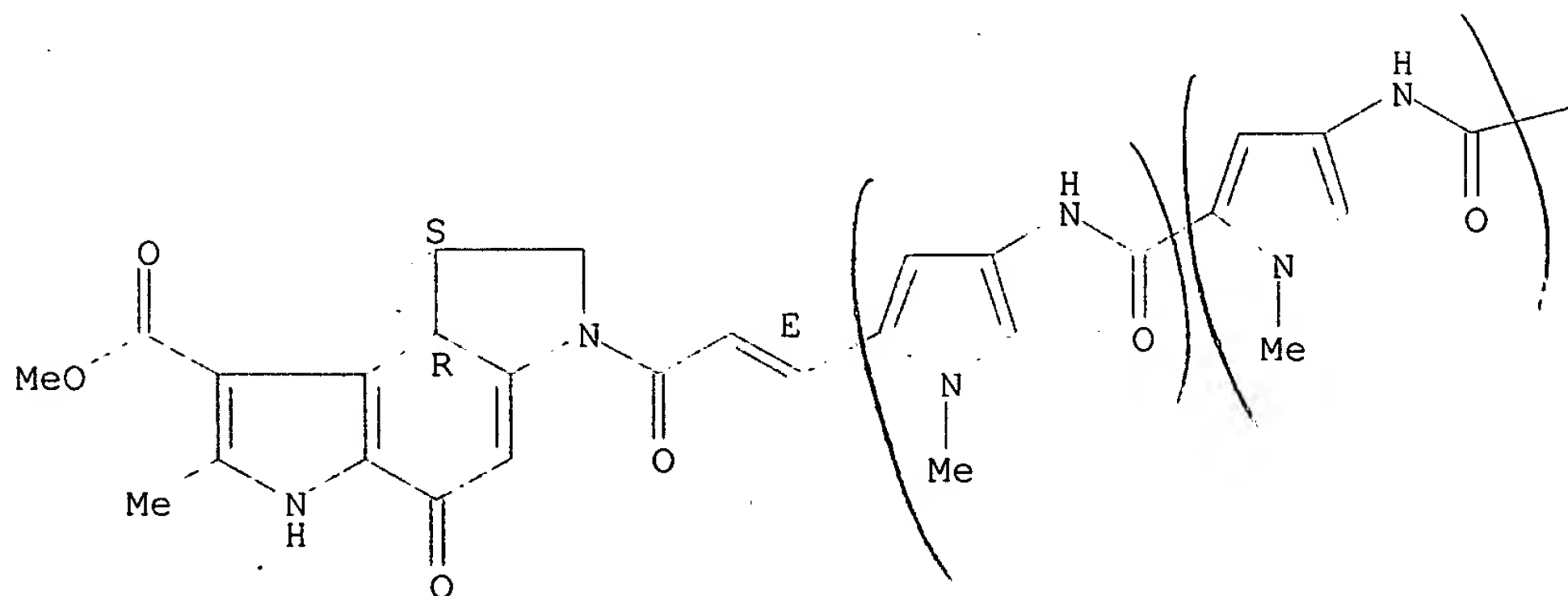
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:275556

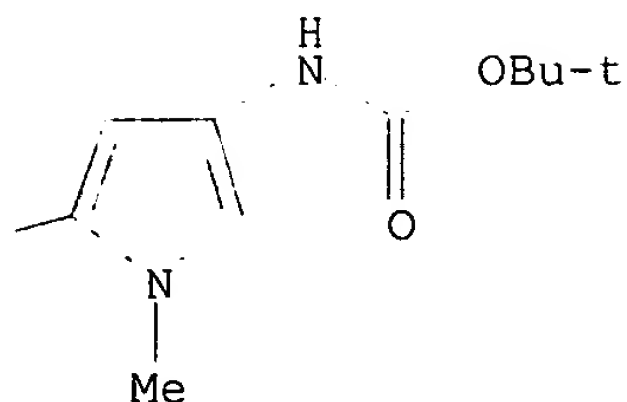
L11 ANSWER 27 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 251999-81-2 REGISTRY
CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-[[[4-[[[1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C39 H42 N8 O8
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

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PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:22791

L11 ANSWER 28 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 251999-80-1 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[(2E)-3-[4-[[[4-
 [(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-
 yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-
 hexahydro-6-methyl-4-oxo-, methyl ester, (7bR,8aS)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C33 H36 N6 O7

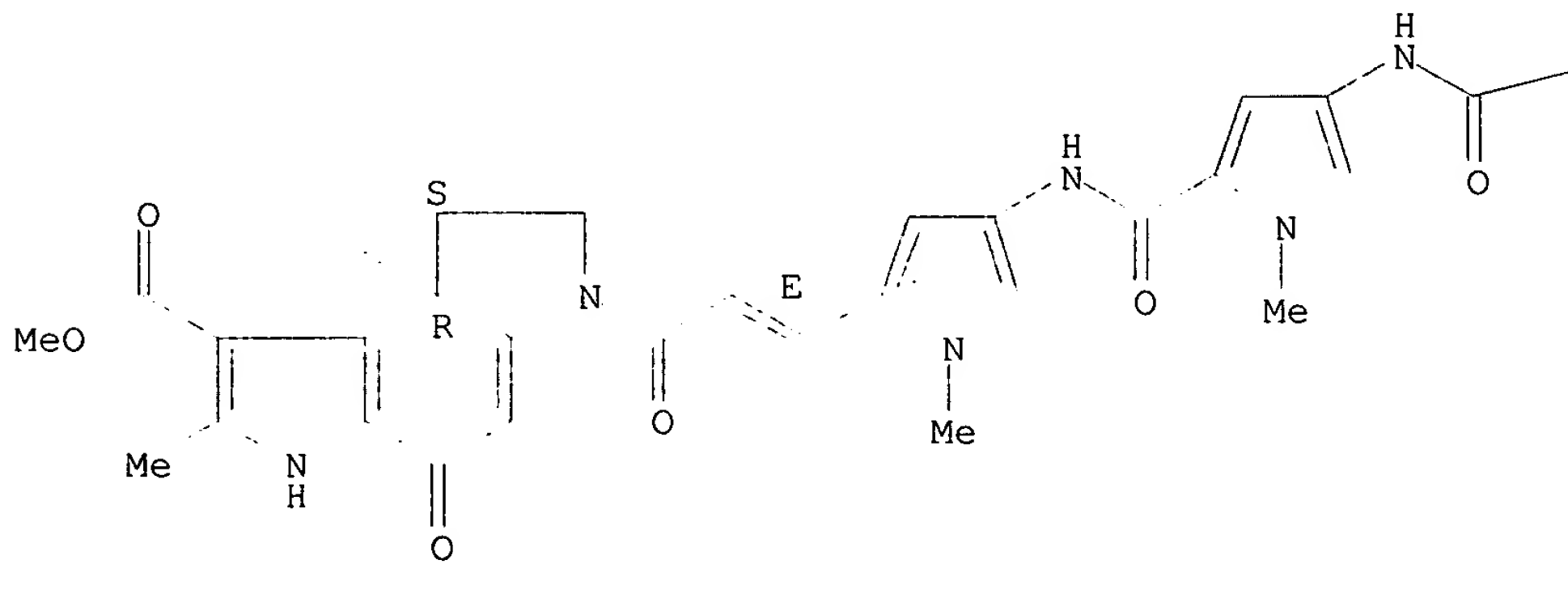
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

Double bond geometry as shown.

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PAGE 1-B

OBu-t

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:22791

L11 ANSWER 29 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 202419-15-6 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-[[[4-
 [[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-
 yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-
 pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-,
 methyl ester (9CI) (CA INDEX NAME)

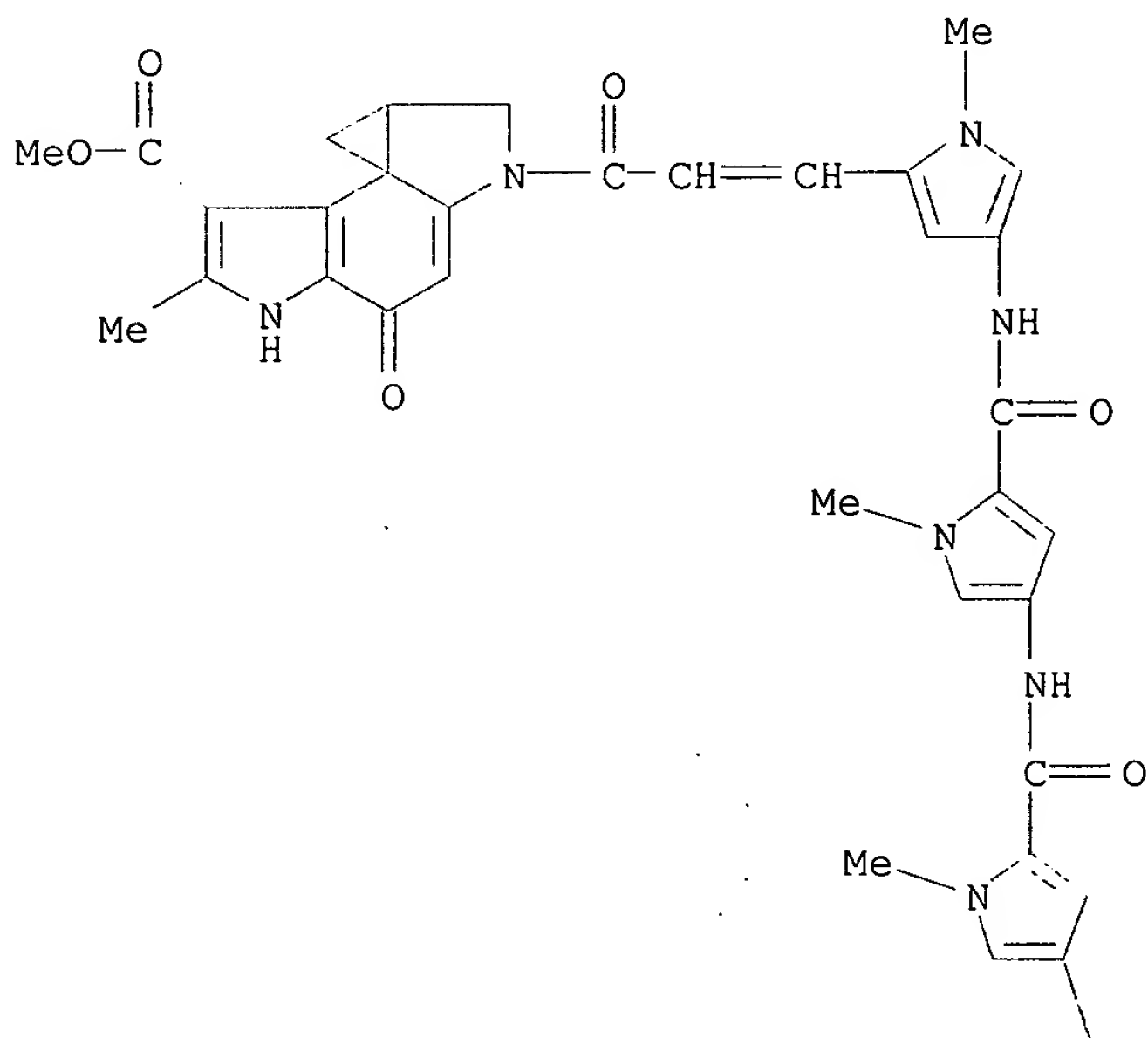
FS 3D CONCORD

MF C39 H42 N8 O8

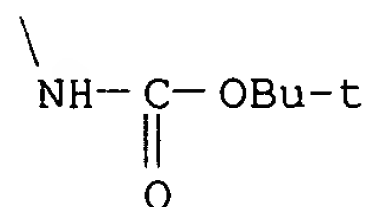
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

PAGE 1-A



PAGE 2-A



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:154100

L11 ANSWER 30 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 202419-12-3 REGISTRY

CN Cyclopropa[c]pyrrolo[3,2-e]indole-7-carboxylic acid, 2-[3-[4-[[[4-[[[4-
 [[(1,1-dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-
 yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-
 pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-,
 methyl ester (9CI) (CA INDEX NAME)

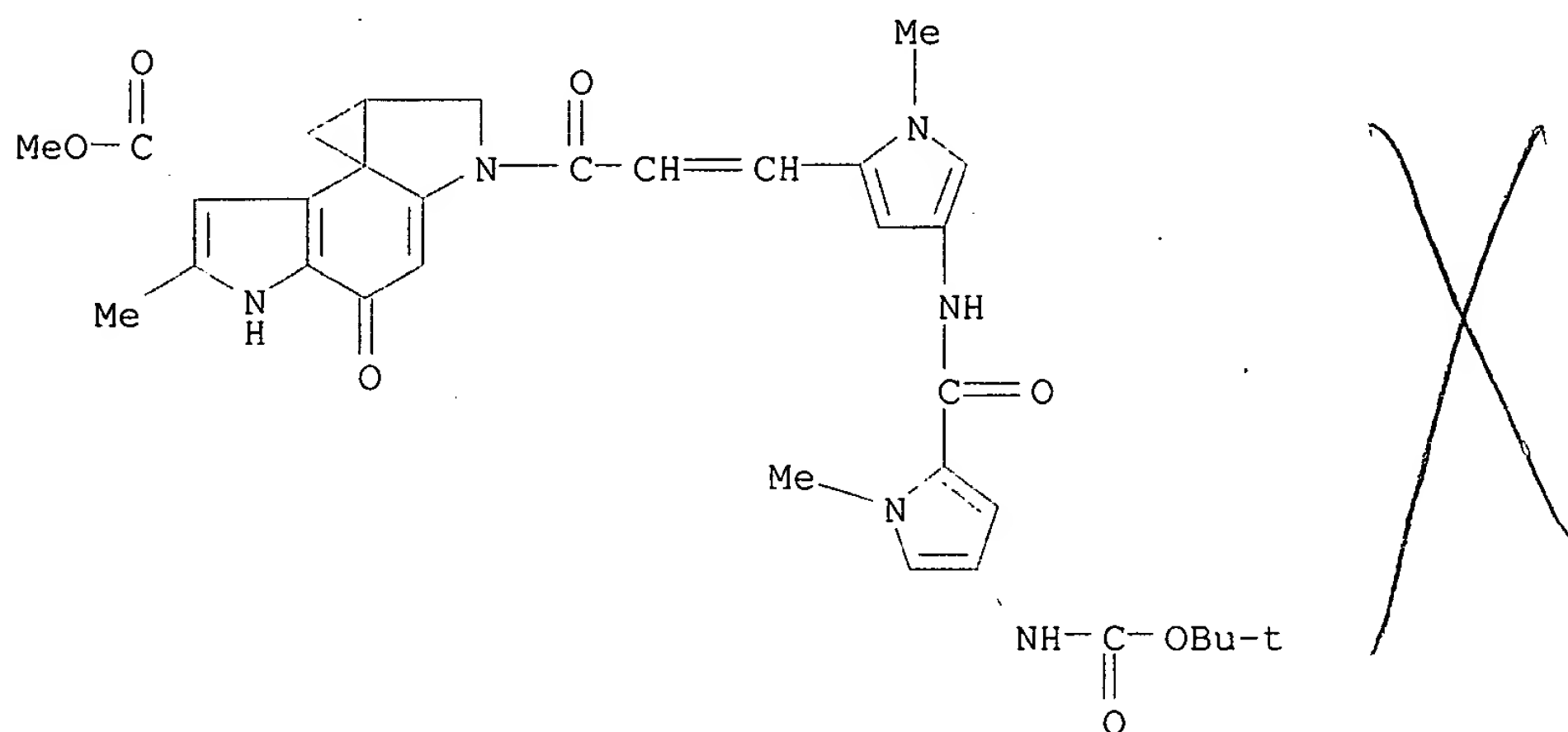
dimethylethoxy)carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]carbonyl]amino]-1-methyl-1H-pyrrol-2-yl]-1-oxo-2-propenyl]-1,2,4,5,8,8a-hexahydro-6-methyl-4-oxo-, methyl ester (9CI) (CA INDEX NAME)

FS 3D CONCORD

MF C33 H36 N6 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 128:154100